UNIVERSITY OF CALIFORNIA

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# The Effect of Methanol on the Mobilization of Tetrachloroethylene in a Water-Saturated Soil Column

A thesis submitted in partial satisfaction of the requirements for the degree Master of Science in Civil Engineering

by

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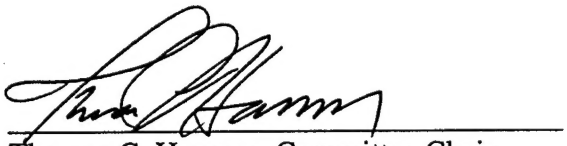

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## Dedication

I would like to dedicate this thesis to my wife May for her unconditional support of my academic pursuit and military career. A special thanks to my parents Ron and Della, and my brother Scott, for all their help. Finally, to my son Brandon, who was born during the preparation of my thesis, for helping me maintain my sense of humor!

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ABSTRACT OF THE THESIS

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Professor Thomas C. Harmon, Chair

The contamination of surface waters and groundwater by chlorinated solvents continues to be a major environmental issue. Today, the challenge to environmental engineers is not necessarily which remediation technique to use, but how to enhance the remediation technique in order to accelerate the clean-up process.

The "pump-and-treat" method for remediating organic contaminants is experimenting with the use of chemical additives to increase the efficiency rate of subsurface contaminant removal. Because of their favorable chemical properties, alcohols such as methanol are often used in conjunction with water to flush a contaminated area, and subsequently pump it to the surface for treatment. For this study,

the objectives were: (1) to reconfirm the impact of a cosolvent, such as methanol, on the observed retardation of nonpolar organic solute (tetrachloroethylene, PCE) transport in a water-saturated porous medium; and, (2) to provide evidence that ineffective mixing of two inhomogeneous fluids, such as methanol and water, can negatively impact the desired cosolvent effect.

For the one-dimensional laboratory column at the flowrate tested (0.745 mL/min), methanol failed to produce the hypothesized cosolvent effect. The degree of retardation of PCE did not decrease log-linearly, but instead showed no significant difference with increasing methanol fraction. Therefore, the column system, under the conditions used in this study, may have been subject to the ineffective fluid mixing potentially associated with cosolvent-water systems. However, breakthrough behavior for methanol was generally symmetric and failed to exhibit any signs of ineffective mixing. The nature of these results underscores the complexity of the problem of mixing of inhomogeneous fluids.

# *Chapter 1. Introduction*

Chlorinated solvents, used as cleaning agents in a vast array of industries, from dry cleaning to aerospace, are known or suspected as either carcinogens or mutagens. The frequent industrial use of these chemicals, such as tetrachloroethylene (PCE), trichloroethane (TCA), and trichloroethylene (TCE), has led to widespread contamination of soil and groundwater. Because of the high volatility of these organic compounds, their concentrations in surface waters, which are only a few micrograms per liter, is not a water quality issue. However, it is in the groundwater where the concentrations of chlorinated solvents will be thousands of times higher since the contaminants cannot volatilize, and hence will tend to remain in water or sorb to soil. Most frequently, the corrective action for subsurface contamination is to flush the contaminated area with water and subsequently pump it to the surface for treatment. This conventional "pump-and-treat" (Mackay and Cherry, 1989) strategy is effective for removal of a majority of the contaminant. Unfortunately, the remaining contaminant is still, most often, well above prescribed limits.

The remaining contamination is often due to nonaqueous phase liquids (NAPLs) in the subsurface. NAPLs are immiscible in water and can have densities that are either greater than water or less than water. When a NAPL has a density greater than water, it is commonly referred to as a dense nonaqueous phase liquid (DNAPL). Conversely, if the NAPL's density is less than water, it is commonly referred to as a light nonaqueous phase liquid (LNAPL). Examples of DNAPLs include chlorinated solvents such as trichloroethylene. Some examples of LNAPLs include gasoline, petroleum oil, and diesel fuel. The continued presence of NAPLs in the subsurface poses a major clean-up problem. It is critical to locate and remove any NAPLs from a hazardous waste site because NAPLs provide a long-term source of pollution due to their low solubilities.

Because of the limitations of the "pump-and-treat" method for remediating NAPL organic contaminants, alternative remediation techniques such as bioremediation and chemical additives are being considered.

## *1.1 Bioremediation*

Bioremediation is the use of microorganisms to degrade subsurface contaminants. The microorganisms, generally bacteria, convert harmful chemical compounds to less harmful chemical compounds in order to effect remediation of a contaminated site. To survive, the microbes require: a carbon supply, an energy supply, and nutrients. The types and amounts of carbon, energy, and nutrients, are part of the overall design of the remediation system. Therefore, a detailed understanding and control of the site hydrogeology is required to implement an efficient remediation effort. Contaminant factors, such as: solubility, volatility, viscosity, and toxicity; and soil conditions, such as: permeability, soil type, depth to groundwater, mineral content, oxidation/reduction potential, and pH; may have a profound affect on the general remediation design.

The key to successful bioremediation is engineering the system such that all the microbe requirements can combine in the subsurface. However, engineering the system is not as simple as one might expect. The geologic medium for remediation must be permeable enough to allow the introduction of energy and nutrients. Many intraparticle pores are too narrow to allow microbe access. If the microbes cannot reach the zone of contamination, the remediation effort will fail. Another limitation to bioremediation is that it is difficult to biostimulate immobile zones. Most often, the contaminant must diffuse out to the biostimulated zone before bioremediation can occur. Finally, bioremediation is still in the developmental stage and there are few documented cases of using bioremediation in the saturated zone.

## *1.2 Chemical Additives*

Enhanced remediation techniques using chemical additives are being introduced to increase the efficiency rate of contaminant removal from the subsurface (Palmer *et al*, 1992; Augustijn *et al*, 1994). In-situ solvent flushing involves injecting a mixed solvent into the subsurface of a site contaminated with organic chemicals. Surfactants, alcohols, or mixtures of these chemicals are often used as the solvent (Imhoff, 1995). When the solvent is in sufficient quantities relative to water, it is often referred to as a water-miscible organic *cosolvent*. Miscibility describes a compound's ability to mix in any ratio with water without separation into two phases, while immiscibility means a compound is unable to mix with water. Because of their favorable chemical properties, alcohols, such as methanol, have been investigated as potential cosolvents.

## *1.3 Thesis Overview*

The objective of this thesis study is to test the ability of methanol as an effective cosolvent. Through a series of experiments, this research will investigate: the transport and dissolution of methanol in a water-saturated porous medium and, the effects of methanol on the mobilization of PCE. The hypothesis of this study is that methanol will decrease the retardation factor of PCE in a porous medium, thereby confirming the impact of cosolvents on remediating hazardous organic compounds.

In Chapter Two, background material relating to organic contaminants will be presented. Chapter Three will delve into the theory of cosolvency and subsurface remediation. In Chapter Four, the research objectives and approach for this thesis will be outlined. Chapter Five will detail the experimental methods used, and Chapter Six will

highlight the results. Finally, in Chapter Seven, a summary of the findings, and the conclusions reached in this study, will be presented.

# *Chapter 2. Background*

Before reviewing the underlying theory of cosolvency, it is instructive to examine background material relating to organic contaminants and their properties, properties affecting the transport of a NAPL-based solute, and physical properties affecting the fate and transport of organic chemicals in groundwater.

## *2.1 Organic Contaminants and their Properties*

Organic contaminants, such as TCE and PCE, are just two of the myriad of chlorinated solvents found in the subsurface. The extent to which these solvents contaminate the subsurface depends, in part, on the properties of the organic contaminants. Polarity refers to the extent of the dipole moment in a molecule. Hydrophobicity is the tendency of organic compounds dissolved in groundwater to adsorb onto solid surfaces. Less polar molecules are more hydrophobic. Solubility refers to the concentration of a species in a saturated aqueous solution. TCE and PCE have low solubilities due to their lack of polarity; hence, they are commonly referred to as hydrophobic contaminants.

## *2.2 Properties Affecting Transport of a NAPL-based Solute*

Several key properties affect the transport of a NAPL-based solute. Solubility plays a major role. Another important property is sorption. Sorption is the term used to describe adsorption and/or absorption when independent determination of the processes is impossible. Adsorption is the net accumulation of a solute at the solid-liquid interface; while absorption occurs when a solute is transferred from one phase (i.e., water) to another, such as soil or organic matter.

## 2.3 *Physical Processes Affecting Fate and Transport of Organic Chemicals in Groundwater*

Organic contaminants may enter the subsurface by spills, leaks, or intentional disposal. In the saturated zone, these organic chemicals will either dissolve in the groundwater or will remain immiscible with groundwater in the form of NAPLs. A review of the physical processes that most strongly influence this phenomena will be presented to assist in the understanding of organic contaminant transport and distribution in the saturated zone.

### *2.3.1 The Advection-Dispersion Equation*

Transport phenomena in the saturated zone is governed by the *Advection-Dispersion* equation (e.g., Freeze and Cherry, 1979):

$$\underset{(1)}{\frac{\partial C}{\partial t}} = \underset{(2)}{\frac{\partial}{\partial x}\left(D_{HD}\frac{\partial C}{\partial x}\right)} - \underset{(3)}{\frac{\partial}{\partial x}\left(v_X C\right)} \qquad (2\text{-}1)$$

where $D_{HD}$ = hydrodynamic dispersion coefficient [$L^2/T$]
$v_X$ = the average pore water velocity [L/T]
$t$ = time [T]
$x$ = distance [L]
C = solution concentration [$M/L^3$]

The first term (1) is the net accumulation. Term (2) represents the transport due to dispersion and term (3) represents the transport due to advection.

A more complete modeling of the transport of the solute in the aquifer would consider the immobile zones in each molecule of porous media. To account for this property of the media the concept of *retardation* will be introduced in Section 2.3.4.

### *2.3.2 Advection*

Saturated-zone transport of dissolved contaminants is due primarily to advection. Advection is the process by which a solute is transported by the movement of the fluid itself (i.e., groundwater flow). The flow of groundwater is driven according to Darcy's Law. It is important to be able to estimate the rate at which groundwater is moving through an aquifer. This rate, the Darcy velocity, can be found by solving for the velocity using Darcy's Law (2-2).

$$Q = - KA \frac{\partial h}{\partial L} \qquad (2\text{-}2)$$

where Q = flow rate [$L^3/T$]
K = hydraulic conductivity or coefficient of permeability [L/T]
A = cross-sectional area [$L^2$]
$\frac{\partial h}{\partial L}$ = hydraulic gradient

The Darcy velocity is not the actual groundwater velocity because the cross-sectional area, given by A in (2-2), of an aquifer is made up of solids. The actual cross-sectional area is much smaller, and hence, the actual groundwater velocity is considerably faster than the Darcy velocity.

Groundwater will flow from points of high piezometric head to points of low piezometric head. The difference in water elevation and pressure head between points determines the hydraulic gradient which drives the flow of groundwater. In gentle topography and under unconfined conditions, the gradient normally follows the topography, and the groundwater flow rate can be estimated within a factor of 10 (Roberts *et al*, 1986). However, several factors, such as a porous media's hydraulic conductivity, can make the determination of the groundwater flow rate quite difficult to

estimate. Hydraulic conductivity is a measure of the ability of a porous media to transmit a fluid (i.e., water) and is dependent on the properties of the porous media and the fluid.

A subsurface porous media found in nature is generally *heterogeneous*; that is, the hydraulic conductivity varies from place to place. The porous media is considered to be *homogeneous* when the hydraulic conductivity is the same throughout. Sometimes hydraulic conductivities are a function of the flow direction. Generally, hydraulic conductivities are higher in the horizontal direction than in the vertical direction (Freeze and Cherry, 1979). Aquifers that have the same hydraulic conductivity in any flow direction are called *isotropic*, while those aquifers in which the conductivities varies according to direction are called *anisotropic*. Because *homogeneous* and *isotropic* aquifers are rarely found in nature, one must collect empirical measurements to obtain reasonably accurate estimates of the groundwater velocity in a flow field.

For one-dimensional soil column experiments, such as the one used for this study, a homogeneous and isotropic aquifer can be simulated. Because a pore water velocity is typically known for this type of system, the flow equation (2-2) is not employed. A one-dimensional, homogeneous and isotropic porous medium will limit variations from occurring. However, the limitation of this lab system is readily apparent in that it is not representative of an actual environmental system.

### *2.3.3 Dispersion*

Dispersion is the tendency of a solute to spread during transport. The two main causes of dispersion are mechanical mixing and molecular diffusion (Freeze and Cherry, 1979). Mechanical mixing is mixing due to velocity gradients. The factors which affect the degree of mechanical mixing include: different sized pore channels within the porous media, variations in pore geometry (tortuosity), and fluctuations in the local flow

velocities relative to the mean flow direction. Molecular diffusion is the net flux of a solute from a zone of high concentration to a zone of low concentration. Dispersion results in the dilution of contaminant pulses and the attenuation of concentration peaks. Therefore, the maximum concentrations diminish with increasing distance from the source (Mackay *et al*, 1985).

Dispersion can occur longitudinally, in the principal direction of flow; or transversely, perpendicular to the principal direction of flow. The hydrodynamic dispersion coefficient is a tensor (Bear, 1972):

$$D = \alpha_L D^1 + \alpha_T D^2 + D^* \qquad (2\text{-}3)$$

where $D$ = hydrodynamic dispersion coefficient [$L^2/T$]
$D^*$ = coefficient of molecular diffusion, which is generally ignored [$L^2/T$]
$\alpha_L$ = longitudinal dispersivity of the porous medium [L]
$\alpha_T$ = transverse dispersivity of the porous medium [L]

For the one-dimensional case,

$$D^1 = v \text{ and } D^2 = 0 \quad \text{where } v = \text{Darcy velocity [L/T]}$$

Therefore,

$$D = \alpha_L (v) \qquad (2\text{-}4)$$

Despite the practical importance of the dispersion process, there is currently no method to confidently predict the magnitude of dispersion for a previously unstudied field situation. For simple hydrogeological systems, the spreading is believed to be proportional to the flow rate. For more complex systems, the dispersivity appears to

depend on the structure of the geologic medium such that it varies with the distance traversed (Mackay *et al*, 1985).

### *2.3.4 Retardation*

Retardation is the apparent slowing of contaminant transport relative to groundwater flow due to sorption. The higher the fraction of the contaminant sorbed, the more retarded is its transport (Mackay *et al*, 1985).

Sorption of halogenated chemicals to soils is a nonspecific combination of two factors. The first factor is related to hydrophobicity. In essence, the molecules are "squeezed out" of the water and deposited on the soil surfaces due to their hydrophobicity (e.g., Curtis *et al*, 1986). The second factor affecting sorption is the fraction of solid organic matter in the aquifer solids, known as organic carbon content. Attempts have been made to correlate organic contaminant sorption with soil organic matter and a chemical property of the contaminant such as the octanol-water partition coefficient (Karickhoff *et al*, 1979). The assumption is that all sorption is due to organic matter implying the amount of sorption is proportional to the amount of organic matter.

If a solute does not sorb to the porous medium, it will move at a velocity equal to the groundwater velocity and, by definition, has a retardation factor equal to one. However, if the solute does sorb to the soil, it will move at a velocity equal to the groundwater velocity divided by a retardation factor, R:

$$R = 1 + \frac{\rho K_d}{\theta} \qquad (2\text{-}5)$$

where $\rho$ = soil bulk density $[M_s/L^3]$
$\theta$ = soil porosity [-]
$K_d$ = equilibrium distribution coefficient $[L^3/M_s]$

The equilibrium distribution coefficient is a function of the soil and the chemical type. Numerous attempts have been made aimed at correlating $K_d$ with chemical properties, such as solubility or octanol-water partitioning coefficient (Karickhoff, 1979; Chiou *et al*, 1983; Curtis *et al*, 1986). These attempts assume that the sorption process is attributed solely to the soils organic carbon fraction. However, other studies (e.g., Ball and Roberts, 1991a) have shown that for soils characterized by low organic carbon contents (i.e., about 0.1% or less w/w), mineral surfaces play a significant role. In any case, the published correlations are best used for a first approximation, and more accurate $K_d$ estimates must be determined experimentally.

## *2.4 Groundwater Remediation*

Contaminated groundwater can contain an abundance of organic chemicals. Due to the low solubility of some of these chemicals, large dilute plumes of contaminant typically appear and propagate through the saturated zone. The most common method of treatment for a contaminated aquifer is a pump-and-treat system. The contaminated groundwater is extracted via a withdrawal well and treated at the surface through a filtration process such as granular activated carbon.

### *2.4.1 Effect of Sorption on Remediation*

In an aquifer, one might expect a contaminant to move at the same speed as the groundwater; however, this is not necessarily the case. Some contaminants are sorbed onto the soil particles thereby reducing the overall solute flow rate relative to that of the groundwater itself. The solute is retarded by a factor R called the retardation factor. For a successful remediation, R pore volumes must be extracted under ideal conditions (assuming the local equilibrium assumption (LEA) applies: no immobile zones and

instantaneous equilibrium is achieved between the water and solid phases). Thus, reducing sorption (or R) would expedite the remediation process.

### *2.4.2 Nonequilibrium Sorption*

Equilibrium sorption models such as LEA assume that the mass transfer rate is fast relative to the flow rate so that equilibrium can be reached. If this is not the case and equilibrium is not attained, a nonequilibrium sorption model is more appropriate. Unfortunately, a kinetic model causes complications at two scales. At the particle scale, mass transfer resistances like intraparticle diffusion can markedly decrease the rate of contaminant release from a sorption site thereby increasing remediation times (e.g., Ball and Roberts, 1991a; Harmon and Roberts, 1994). At the layer scale, an increase in the degree of hydraulic conductivity due to heterogeneity (larger scale immobile or low flow zones) can be a dominant factor in causing remediation times to increase (Rabideau and Miller, 1994; Kong and Harmon, 1996).

### *2.4.3 Effect of Cosolvents on Retardation*

At the particle scale, complications caused by nonequilibrium sorption can be mitigated by the use of cosolvents (Brusseau *et al*, 1991). Cosolvents can lower retardation factors and increase mass transfer rates. This thesis will examine the capacity of a cosolvent to lower the retardation factor of PCE. Before examining the Research Objectives and Approach, Cosolvency Theory and Subsurface Remediation will be reviewed in detail in the next chapter.

# *Chapter 3. Cosolvency Theory and Subsurface Remediation*

The idea of using cosolvents to accelerate the remediation of soils and groundwater has recently been considered for field testing (Augustijn *et al*, 1994). Although a relatively new remediation technique for soil and groundwater, the technology was actually developed in the petroleum industry. The mechanisms involved in cosolvent flooding for enhanced oil or nonaqueous phase liquid (NAPL) recovery have been discussed in several reviews (Reed *et al*, 1977; Larson *et al*, 1982; Lake, 1983; Imhoff *et al*, 1995). Other studies have indicated that the use of cosolvents will reduce the retardation factor substantially, thereby vastly reducing the remediation times (Yalkowsky *et al*, 1981; Rao *et al*, 1985; & Nkedi-Kizza *et al*, 1989).

## *3.1 Methanol as a Cosolvent*

Methanol is a colorless, polar chemical that is miscible with water. Today, methanol has many industrial and consumer uses. Approximately 70% of the methanol produced worldwide is used in chemical syntheses (Ullman, 1990). The most readily apparent use of methanol is as an energy source. The oil crisis in the early 1970's set in motion the need to find alternative sources of fuel. Coupled with the added emphasis on air quality, methanol and methanol-petroleum fuel mixtures were a good solution. As the 21st century approaches, the use of methanol is increasing. Because of methanol's low freezing point and miscibility with water, it is sometimes used in refrigeration systems. Moreover, it is used as an anti-freeze or an absorption agent in gas scrubbers.

Methanol is an excellent choice for a cosolvent. Recent studies (e.g., Imhoff *et al*, 1995) cite methanol's advantages: (1) it is relatively inexpensive; (2) once diluted to low concentrations in groundwater, it is readily biodegradable; and (3) it is representative of a class of alcohols that do not significantly partition into denser than water nonaqueous

phase liquids (DNAPLS), and thus will not enhance downward DNAPL migration by reducing the interfacial surface tension of the DNAPL residual ganglia.

## *3.2 Cosolvent Theory*

The idea of including other organic molecules in water to affect the solubility of organic contaminant in a solution is the basis behind the theory of cosolvency. When the organic molecules are present in relatively large quantities ($\cong >$ 10% volume/volume), they act as solvent molecules themselves and partially surround the solute of interest, approximately in proportion to their volume fraction in the solution (Yalkowsky *et al*, 1976). If the organic molecules are not present in these quantities, the effect on solubility ranges from *no effect* (for < 0.001 v/v) to a *slight effect* (for > 0.001 but < 0.10).

Yalkowsky *et al* (1976) postulated that the excess free energy of solution of a solute in a water organic cosolvent mixture should be a linear combination of the solute's excess free energies of solution in each solvent alone. Part of the organic solute is dissolved in water and the remainder of the organic solute is dissolved in the organic cosolvent. By solving for the excess free energy of solution in pure water and the excess free energy of solution in the cosolvent, and by substitution, Yalkowsky *et al* (1976) showed mathematically that the log solubility of a solute increased linearly as the fraction of cosolvent in the solution mixture increased. This result was well supported by experimental observations conducted by Yalkowsky *et al* (1976) using a series of aromatic hydrocarbons.

## *3.3 Cosolvent (Methanol) Effects*

A recent study (Imhoff *et al*, 1995) investigated the following topics: (1) the effect of methanol on various system parameters; (2) the influence of methanol on phase

partitioning; and, (3) the effect of methanol on PCE mobilization and rate of PCE dissolution. Conclusions were made after conducting a series of batch-contacting and generator column experiments.

### *3.3.1 Physical and Chemical Properties of PCE*

The effect of methanol on various physical and chemical properties of PCE were determined for a select number of methanol/water volumetric fractions (0%, 20%, 40%, and 60% methanol by volume). The 60% methanol by volume results demonstrated that methanol significantly affected: the viscosity of the aqueous phase, the interfacial tension between the aqueous phase and PCE, the molecular diffusion coefficient of PCE, and most markedly, the PCE solubility. As their study (Imhoff *et al*, 1995) pointed out, an increased molecular diffusion coefficient and an increased solubility resulted in a faster remediation time.

### *3.3.2 Mobilization of PCE*

Three column experiments were conducted to examine the effect of various methanol/water mixtures on the mobilization of trapped PCE ganglia (Imhoff *et al*, 1995). Although column experiments one and three resulted in no measurable PCE mobilization, experiment two demonstrated PCE mobility. The injection of a 60% methanol/water mixture into the column increased the aqueous phase viscosity, decreased the nonaqueous-aqueous phase interfacial tension, and increased the density difference between the nonaqueous and aqueous phases. It was readily apparent in the analysis of experiment two that the flushing of the column with the methanol cosolvent may have enhanced the downward migration (mobilization) of DNAPL ganglia.

### *3.3.3 Dissolution and Mass Transfer Rate Coefficient*

Imhoff *et al* (1995) demonstrated that various methanol/water mixtures had an impact on the rate of PCE dissolution and the solubility limit of PCE in the aqueous phase. The change in the mass transfer rate coefficient with varying methanol fraction was due to the corresponding change in aqueous phase viscosity. When plotting the maximum potential mass flux versus the methanol fraction, the maximum potential mass flux was shown to increase by a factor of 30 as the methanol/water fraction increased from 0% to 60%. The improvement in the mass flux was attributed to the increase in aqueous phase PCE solubility.

### *3.3.4 Related Research*

There are several publications on the effective use of cosolvents for enhanced in situ remediation. The major conclusions from these are briefly summarized in this section.

*Nkedi-Kizza et al (1985)* presented data in their study that clearly demonstrated the validity of the solvophobic approach for predicting the sorption of hydrophobic organic chemicals (HOC's) from binary solvent mixtures. They concluded that for each sorbate, the sorption coefficient decreased log linearly as the fraction of organic cosolvent increased.

*Fu et al (1986)* studied the hydrophobic sorptive behavior of four aromatic solutes onto three different soils with solvent/water mixtures. For a polar solvent, sorption decreased semi-logrithmically with an increase in volume fraction of solvent in the aqueous phase. This may have been the result of the solvent/water mixture swelling the organic carbon associated with the soil and thereby increasing solute accessibility to

organic matter. The conclusion of the study was that the more hydrophobic the solute, the greater the effect of solvent in solvent/water mixtures on solute solubility enhancement, and hence the less the tendency to sorb onto soil. Thus, the results of this investigation were particularly significant for those aromatic solutes exhibiting the lowest aqueous phase solubility.

*Rao et al (1990)* demonstrated that the presence of a completely miscible organic solvent (CMOS) increases the partially MOS solubility which in turn, is reflected in increased solubility and decreased sorption of hydrophobic organic chemicals (HOC's). Further, with increased volume fraction of a CMOS in a binary mixed solvent, HOC solubility increased and sorption decreased, essentially in a log-linear matter. They concluded that an increase in HOC solubility in the presence of cosolvents was reflected by decreased sorption by soils and increased mobility of HOC's.

*Augustijn et al (1994)* demonstrated in laboratory miscible displacement experiments that the smaller the retardation factor in water and the higher the cosolvent fraction, the faster the contaminant was recovered by solvent flushing. In addition, the presence of non-equilibrium conditions, soil heterogeneity, and the type of cosolvent influenced the time required to recover the contaminant. Augustijn *et al* found that solvent flushing was appropriate for more hydrophobic chemicals. Experimental data and model simulations showed that with increasing cosolvent content, the contaminant eluted at higher concentrations, thus improving the contaminant recovery efficiency. The conclusion of the study was that high cosolvent fractions were most effective for the elution of contaminants. The recovery efficiency was expected to decrease under non-equilibrium conditions and in a heterogeneous soil. The type of cosolvent and composition of the solvent mixture are design parameters that can be used to optimize the recovery efficiency.

*Harmon et al (1994)* focused on two aspects of methanol's behavior in the subsurface environment: (1) the mixing and dissolution; and, (2) the mobilization of sorbing organic contaminants. The studies were carried out in batch and column systems composed of a well-characterized sand fraction. All systems were water-saturated. The study examined: the impact of methanol on the sorption of the hydrophobic contaminant, benzene; the transport of methanol and benzene as solutes; the mixing behavior of methanol in a water-saturated soil column; and the impact of methanol mobilizing benzene in a water-saturated soil column. The results of the experiments showed that the retardation factor of benzene (i.e., sorption) decreased with increasing methanol fraction. However, at higher methanol fractions (>20%), there was an apparent increase in the retardation factor. They attributed the increase in retardation to the density difference between water and methanol. The major conclusions generated by the study were: (1) methanol reduces the equilibrium transport parameter (confirming results from previous studies); and (2) accurate modeling of the mixing of pure methanol with water in porous media requires addressing the water-methanol density differences.

### *3.3.5 The Mixing of Miscible, Inhomogeneous Fluids in the Subsurface*

A major finding of the Harmon *et al* study (1994) was that there was a relatively poor understanding of the dynamics of mixing of miscible, inhomogeneous fluids in the subsurface environment. They found that the differences between methanol and water (i.e., density and viscosity) imply that the displacement of one fluid by the other will defy conventional flow and transport modeling approaches, which treat density and viscosity as constants. Currently, research is under way by Harmon *et al* (1996) to illustrate the dynamics of mixing and transport of miscible, inhomogeneous fluids in a porous medium

in hopes of increasing the understanding of, and design capabilities for, chemically enhanced remediation.

## *3.4 Thesis Objectives*

The study by Harmon *et al* (1994) is the basis for this thesis. The impact of methanol as a cosolvent will be further investigated; in this case, on the nonpolar organic solute, PCE. Furthermore, this study will investigate the mixing dynamics of miscible, inhomogeneous fluids (methanol and water) in the context of soil and groundwater remediation strategies.

# *Chapter 4. Research Objectives and Approach*

As with the previous study (Harmon *et al*, 1994), the research approach for this masters thesis focuses on the study of a one dimensional, single aquifer solid type. However, the organic contaminant to be used in conjunction with methanol is PCE instead of benzene.

## *4.1 Research Objectives*

The objectives of this study were two-fold:

(1) To reconfirm the impact of a cosolvent (i.e., methanol) on the observed retardation of nonpolar organic solute PCE transport in a water-saturated porous medium.

(2) To provide evidence that ineffective mixing of two inhomogeneous fluids (i.e., methanol and water) can negatively impact the desired cosolvent effect.

## *4.2 Experimental Approach*

The porous media used in this study is Borden sand (-40+60 U.S. Standard mesh size, mean particle diameter = 0.33 mm). The experiments performed in the study were:

(1) Tracer Experiments- Breakthrough curves of trace amounts of $^{14}C$-labeled methanol/PCE in water to examine their transport behavior.

(2) Methanol Displacement Experiments- A series of breakthrough curves for examining the transport of various methanol fractions through the sand column.

(3) PCE Mobilization Experiments- A series of breakthrough curves to observe methanol mobilizing PCE in a saturated soil column.

## *4.3 Theoretical Approach*

The results obtained from these experiments were modeled using available analytical solutions to the advection-dispersion equation. In the tracer experiments, trace amounts of MeOH in water were run through the column. The goal was to generate breakthrough curves which would provide a basis of comparison for the methanol displacement experiments and PCE mobilization experiments.

In the next set of experiments, the goal was to determine the advection and dispersion characteristics of methanol as a solute and as a cosolvent. Five individual tests were conducted. The methanol fractions used for each of the test pulses were 1%, 5%, 10%, 20%, and 50%. Using the soil-column lab set-up discussed in Chapter Five, forty experimental data points were measured in each test and used to characterize a specific methanol breakthrough curve. A least-squares fitting program, CFITM, (van Genuchten, 1981) was used to find the Peclet number for each data set assuming a retardation value of one. CFITM is a FORTRAN program capable of solving the nondimensional form of the Linear equilibrium adsorption (LEA) model (LEA model discussed in Section 5.1). With a Peclet number for each methanol fraction, the stage would be set for the next set of column experiments.

In the final set of experiments, the goal was to determine how the different methanol fractions would affect the mobilization of PCE in the soil column. Using the same experimental set-up, forty experimental data points were measured for each methanol fraction. Using the Peclet number generated from the previous set of experiments, CFITM was used to fit the retardation factor. The fitted retardation factor would be an indication of methanol's ability to mobilize PCE.

# *Chapter 5. Modeling Approach and Experimental Methods*

## *5.1 Modeling Approach*

Transport of a nonsorbing solute in a one-dimensional water-saturated porous medium is governed by the advection/dispersion equation (e.g., Freeze and Cherry, 1979):

$$\frac{\partial C}{\partial t} = D_{HD} \frac{\partial^2 C}{\partial x^2} - v_X \frac{\partial C}{\partial x} \qquad (5\text{-}1)$$

where $D_{HD}$ = hydrodynamic dispersion coefficient [$L^2/T$]
$v_X$ = the average pore water velocity [L/T]
$t$ = time [T]
$x$ = distance [L]
C = aqueous concentration [$M/L^3$]

Equation (5-1) assumes steady-state flow and no interactions between the aqueous phase and the solid phase.

If chemical adsorption is considered, an additional term is needed to account for the interaction between the aqueous phase and the solid phase and the advection/ dispersion equation becomes:

$$\frac{\partial C}{\partial t} = D_{HD} \frac{\partial^2 C}{\partial x^2} - v_X \frac{\partial C}{\partial x} - \frac{\partial S}{\partial t} \qquad (5\text{-}2)$$

where S = adsorbed concentration [M/M].

Prior to the conception of the CFITM model, significant deviations were observed between the calculated and experimental effluent curves using equation (5-2). In an

attempt to account for these apparent differences, several models were introduced (for review, see Harmon *et al,* 1989). The increasing complexity with which the immobile zones were viewed (described by the S term) led to CFITM. (van Genuchten, 1981).

In his program CFITM, van Genuchten (1981) considers five conceptual models. Depending on the exact form of the transport model, the program allows up to five different parameters to be estimated simultaneously. The least-squares computer model fits these transport parameters to column effluent data. The five transport models are:

Model A: Linear equilibrium adsorption

Model B: Physical non-equilibrium

Model C: Physical non-equilibrium in the presence of anion exclusion

Model D: Two-site kinetic non-equilibrium adsorption

Model E: One-site kinetic non-equilibrium adsorption

The model used for this work is the Linear Equilibrium Adsorption Model (LEA). With the LEA model, the relationship between the aqueous concentration and the sorbed concentration is described by a linear isotherm:

$$S = K_d C \qquad (5\text{-}3)$$

where $K_d$ is an empirical distribution coefficient [$L^3/M_s$]. Substitution of equation (5-3) into equation (5-2) yields the following transport equation:

$$R \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v_x \frac{\partial C}{\partial x} \qquad (5\text{-}4)$$

where R is the retardation factor [-] equal to:

$$R = 1 + \frac{\rho K_d}{\theta} \qquad (5\text{-}5)$$

where $\rho$ = soil bulk density [$M_s/L^3$]
$\theta$ = soil porosity [-]
$K_d$ = empirical distribution coefficient [$L^3/M_s$]

The program requires input data for the following dimensionless variables in order to perform the analysis of the effluent data:

(1) Length (Z) = $x/L$ L = length of porous media

(2) Concentration (C) = $C/C_o$ $C_o$= influent concentration

(3) Pore volumes (T) = $v_x t/ L$

(4) Peclet Number (P) = $v_x L/ D_{HD}$

For the dimensionless parameter (4), the Peclet number is defined as the ratio of advective flux to dispersive flux. A high Peclet number means advection is dominating transport while a low Peclet number implies dispersion is dominating transport. Typical Peclet number values for natural flow in groundwater ranges from one to five; however, these values may be greater under pumping conditions (Mackay *et al*, 1985).

To use van Genuchten's model, one must input the Peclet number, the retardation factor, the length of the input (pulse), and the data points (in dimensionless form). The user can request the program to fit one, two or all three parameters (Peclet number, retardation factor, and length of input). The fitted parameters are obtained by means of a

least-squares fit of the appropriate analytical solution to column effluent data. By iteration, a fitted solution is obtained. The non-linear least squares analysis output gives the fitted parameter value and a 95% confidence interval of the results. Although relatively old (1981), van Genuchten's program is not obsolete. The program is versatile and can be dimensioned for up to 90 data points. The least-squares computer model provides a convenient, efficient, and accurate means of fitting various transport parameters to column effluent data (van Genuchten, 1981).

## *5.2 Model Boundary Conditions*

Analytical solutions of equation (5-4) exist for several sets of initial and boundary conditions. In van Genuchten's study (1981) for the LEA model, the initial condition is:

$$C(x,0) = C_i \qquad (5\text{-}6)$$

Two different conditions can be applied to the upper boundary of the soil column (x = 0): a first-type, constant concentration boundary condition of the form:

$$C(0,t) = C_o \qquad (5\text{-}7)$$

or a second-type, constant flux boundary condition of the form:

$$\left(-D \frac{\partial C}{\partial x} + vc\right)\Big|_{x=0} = v\,C_o \qquad (5\text{-}8)$$

where $C_o$ is the concentration of the input solution.

For the lower boundary, the following condition is applied:

$$\frac{\partial C}{\partial x}(\infty,t) = 0 \qquad (5\text{-}9)$$

This condition assumes the presence of a semi-infinite soil column. An alternative boundary condition, one that is frequently used for column displacement studies, is that of a zero concentration gradient at the lower end of the column:

$$\frac{\partial C}{\partial x}(L,t) = 0 \qquad (5\text{-}10)$$

where L is the column length.

In van Genuchten's study (1981), equations (5-9) and (5-10) are both used. However, only the solutions for a semi-infinite medium are included in the curve-fitting program. Because of the relatively small influence of the imposed mathematical boundary conditions, the solutions for a semi-infinite system provide close approximations for those applicable to a physically well-defined finite system, especially for not too short laboratory soil columns.

## *5.3 Experimental Methods*

Each of the experiments summarized in Chapter 4.3 is described in detail in the following section.

### *5.3.1 One-Dimensional Column Set-up*

The set-up of the soil column experiments is shown schematically in Figure 5-1. The controlled flow of methanol and water was driven through the soil column using a quarternary high performance liquid chromatography (HPLC) pump (Paramus, NJ) in

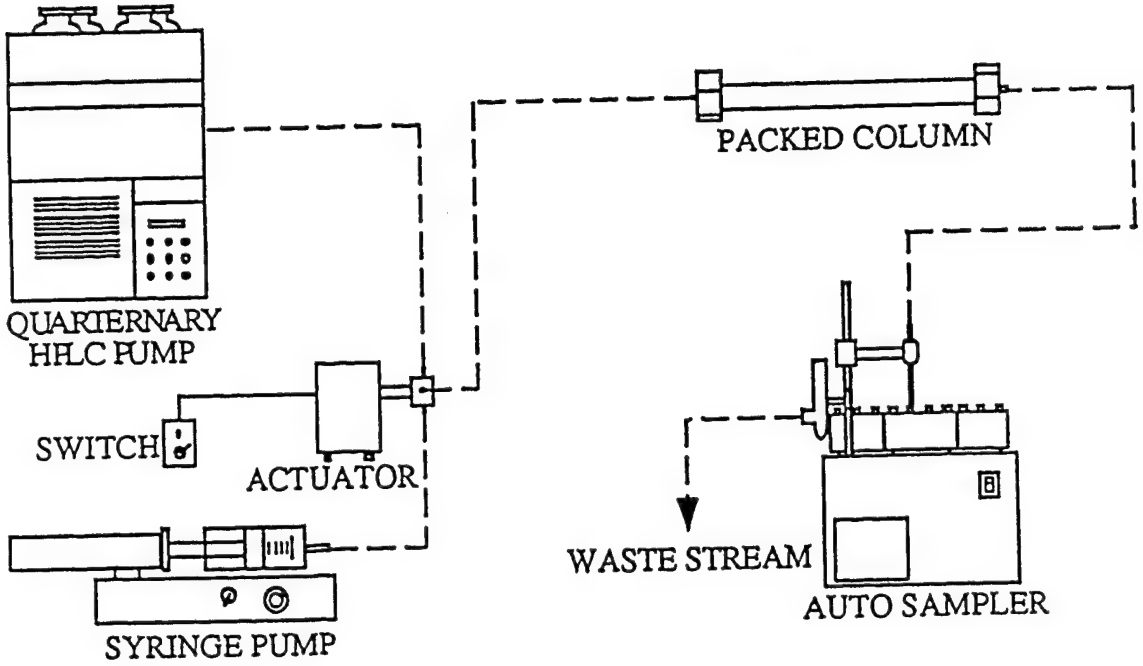


Figure 5-1. Schematic diagram of column study experimental set-up

order to deliver precise mixtures of methanol and water. In this study, a 25-cm steel column (2.06 cm inner diameter) was used, packed with -40+60 (U.S. Std. Mesh Size) Borden sand, which had been examined in particle characterization and organic contaminant sorption and desorption studies with PCE (Ball *et al*, 1990; Ball and Roberts, 1991a; 1991b; Harmon and Roberts, 1994). The Borden sand has: a mean grain diameter of 0.33 mm; a density of 2.71 g/cm$^3$; and an organic carbon content of 0.00023% (Ball *et al*, 1990). The porosity was approximately 0.35. The $^{14}$C-labeled solute, either methanol or PCE, was injected via a gastight syringe mounted on a syringe pump (Sage Model 341B, Boston, MA). A three-way, electronically actuated valve (Valco, Houston, TX), which allowed precise switching between the HPLC pump and the syringe pump, was used for inputting the $^{14}$C-labeled solute pulse. The data points for the effluent breakthrough curves were captured in a series of vials containing liquid scintillation cocktail fluid. All fittings were composed of glass, Teflon, and stainless steel to avoid interactions between the organic contaminants and the apparatus.

### *5.3.2 Analytical Methods*

#### *5.3.2.1 Liquid Scintillation Counting*

Liquid scintillation vials typically contained 5 mL of liquid scintillation cocktail (Insta-gel, Packard Instrument Co., Downer's Grove, IL). The samples were counted with a Packard Tricarb Model 4530 scintillation counter (Packard Instrument Co.). All samples were counted two times for 20 minutes each. Measured counts per minute were converted to actual disintegrations per minute by the external standard method, with quenching efficiencies estimated by a channels ratio method incorporated into the system software. Quenching was less than 5% for all samples and in a spectral region where

quenching was relatively insensitive to changes in solution matrix. Each set of vials to be counted was accompanied by a blank sample (containing 5 mL of scintillation cocktail), used to subtract out background activity.

#### *5.3.2.2 Gas Chromatography*

Prior to each spiking session, the overall (labeled and non-labeled) concentration of the spiking solution was determined by comparison with standard solutions using gas chromatography. Samples of the spiking solution were prepared by extracting approximately 3 mL of the spiking solution with 0.5 mL pentane in 2 mL vials equipped with teflon-lined silicon septa and plastic screw-top caps (Alltech Assoc., Deerfield, IL). Samples and standards were also spiked with an internal standard (1-chloro, 2-bromopropane). The PCE and internal standard were extracted into the pentane during 30 minutes of agitation on a shaker table.

The gas chromatograph, a Hewlett-Packard 5890A, was equipped with a capillary column. The column was followed by a $^{63}Ni$ electron capture detector (ECD). The splitting valve was used on occasion to test the purity of new purchases of radiochemicals. The valve provided the capability of diverting most of the flow (99%) away from the detector in these instances, when a relatively concentrated and radioactive injection was applied. For quantitative purposes, 2-7 μL injections of the pentane were applied, and much less of the flow (<5%) was diverted from the detector. The carrier and makeup gases were helium and Argon/Methane, respectively. The system operated at 150 degrees Celsius, with the detector slightly higher-- 160 degrees Celsius.

#### *5.3.2.3 Radiochemical Purity*

Prior to spiking procedures, spiking solutions were routinely analyzed for volatile impurities via the gas chromatography procedures described in the preceding section. No extraneous peaks were detected in analyses with the PCE spiking solutions.

Spiking solutions were routinely tested for $^{14}C$-nonvolatile and $^{14}C$-$CO_2$ fractions using an acid/base purging procedure (Lanzarone and McCarty, 1988). The nonvolatile impurities, which were not identified, were found to represent approximately 1-2% of the activity, for the PCE. This fraction appeared to remain in the aqueous phase (i.e., did not sorb) in samples for which the A-B-N test was performed prior to purging. No significant fraction of $^{14}C$-$CO_2$ was detected in the PCE spiking solutions. The equilibrium measurement of the sample supernatant was adjusted downward to account for the nonvolatile fraction.

### *5.3.3 Column Experiment Protocol*

#### *5.3.3.1 Preliminary Preparation*

Calibrate the scintillation counting machine (Beckman LS600, Fullerton, CA). At the quarternary HPLC pump, fill the water tank with distilled water (reservoir B) and fill the methanol tank with methanol (reservoir C). Degas the water and methanol tanks with helium for a 1/2 hour. Turn on helium gas at main tank valve and the brass toggle valve that branches to the Teflon tubing to the quarternary HPLC pump. Turn on the helium flow at the pump and get a flow of helium bubbles in the reservoirs. During degassing, continue lab preparation. Label vials (1 through 40) and fill with 5 mL of scintillation cocktail. Record the weight of each of the 40 vials before the experiment begins.

### *5.3.3.2 Solute Preparation*

Retrieve the $^{14}C$-labeled PCE or the $^{14}C$-labeled methanol sample from the refrigerator and allow the sample to equilibrate at ambient temperature. A glass syringe (Hamilton, Reno, NV) was used to load 10 μL of PCE (or 50 μL of methanol) into the 10 mL syringe pump (filled with degassed water or precise methanol/water mixture). Preliminary tests indicated that these amounts were sufficient solute inputs. All syringes should be cleaned using a double-acetone wash procedure after each use. Mix the $^{14}C$-labeled solute input (10 mL syringe pump spiked with radio-labeled PCE or radio-labeled methanol) over a magnetic mixer. Replace sample caps with new teflon caps.

Find $C_o$ (initial concentration in syringe pump). Using three vials labeled A, B, and C; manually, via a syringe, load 5 μL of the radio-labeled 10 mL sample into each of the three vials. Cap and shake immediately. This procedure is performed three times (A, B, & C) to account for possible non-uniform mixing in the syringe pump. Clean the syringe with the double-acetone wash procedure after each sample: A, B, & C. Using the counting machine, obtain a "quick dpm (disintegrations per minute) count" on A, B, & C vials to verify a uniform $C_o$. A "quick dpm count" means the counting machine, using a smaller sample time, will give a dpm count that still maintains a relative error that is less than 2%. The initial concentration is calculated by finding the average of the concentrations of A, B, and C.

When the three counts are within 5% of each other, proceed with the experiment. Set the quarternary HPLC pump to the desired flow rate (0.745 ml/min) and desired methanol/water mixture (0%, 1%, 5%, 10%, 20%, or 50%). Load empty vials 1 through 40 in the auto sampler (Isis Autosampler, Lincoln, NE). Load about three rows of empty test vials in the auto sampler. Set sample and wash times on the auto sampler (i.e., 20 seconds sample interval and one minute 35 seconds wash time).

#### *5.3.3.3 Lab*

Record start time of the experiment. Actuate the syringe pump to load the step input into the column. When the syringe is completely empty, turn-off syringe pump, switch the actuator, and engage the quarternary HPLC pump. Note the time the pulse was stopped. This is the length of the step input. Note the time when the supply of test vials is exhausted and the time when the first recorded sample is taken.

While the experiment is in progress, monitor the quarternary HPLC pump for stoppages. Note the time of any mishaps during the experiment run. Continue to sample the remaining 39 vials. Cap and shake each vial after every sample is taken. Rinse sample tube after each sample vial is taken using distilled water. At the end of the experiment, note the time of completion. After the last sample, turn off the auto sampler while the sampling rod is in the washing tube.

#### *5.3.3.4 Post-Lab*

Weigh each of the 40 sample vials. Load the A, B, C vials and the 40 sample vials into the scintillation counter. Program the counting machine to count the dpm's (ten minute counting time, twice each vial). The packed column must be flushed completely with degassed water before another experiment is run (preferably the next day). When flushing the column, ensure the packed column is in the vertical position. Turn off helium sources at the HPLC pump and the helium tank. Turn off all machines. Clean-up counters and police the area.

### *5.4 Data Reduction*

The data from the scintillation counter will give the "dpm count" for each of the sample vials. The "dpm count" is a mass measurement. To be used in the CFITM model,

the mass measurement must be converted to a concentration measurement. Each "dpm count" will be divided by the difference between the final and initial weights of each corresponding sample vial. The difference between the final and initial weight of each sample vial is in the units of grams. To convert this difference measurement to mLs, divide by the density of water (≅ 1 g/mL). The "dpm/mL" measurement is now in concentration (aqueous) units. All data reduction spreadsheets are included in Appendix A, Column Run Spreadsheets.

## *5.5 CFITM Model Input*

The data input for the model for each sample vial is equivalent "pore volume" [-], and corresponding sample concentration (in [dpm/mL]; as calculated in section 5.4). CFITM provides a least-squares fit for each experimental data point. This output, when connected, is the fitted curve for the column effluent data.

The CFITM data input files for each of the column runs is shown in Appendix B, CFITM Data Input.

## *5.6 Expected Shape of Breakthrough Curves*

The processes affecting solute transport in the saturated zone are advection and hydrodynamic dispersion. Advection would carry the dissolved chemical with the groundwater flow. In an ideal porous media, it would produce close to "plug flow" behavior. Hydrodynamic dispersion would cause the dissolved chemical to spread throughout the porous media. The curves in Figure 5-2 show the shape of the expected breakthrough curve given a square pulse input of solute.

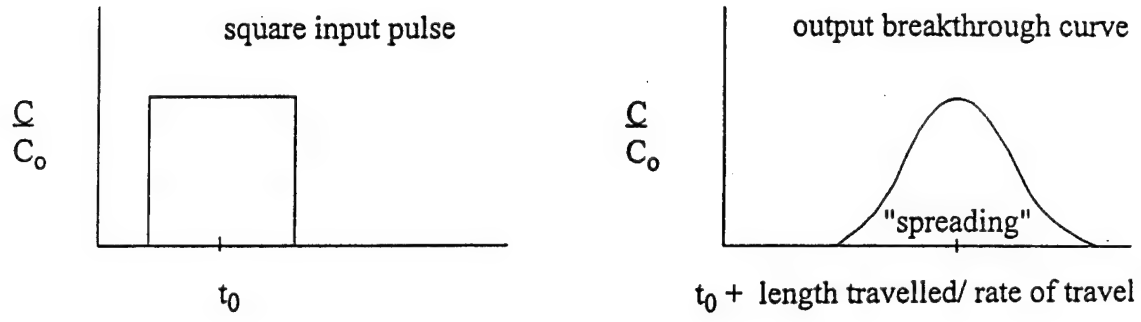


Figure 5-2. Expected output breakthrough curve given a square input pulse.

In Figure 5-2, $t_0$ is the corresponding time for the center mass of the square input pulse. The degree of "spreading" in the output breakthrough curve varies according to the amount of hydrodynamic dispersion. As shown on the time-scale of the output breakthrough curve, the arrival time of the peak is a function of the length of and the rate at which the input pulse travels.

# *Chapter 6. Results and Discussion*

## *6.1 Overview*

Specific results are described in the following sections. Section 6.2 presents column breakthrough data for the miscible displacement tests; that is, employing methanol or PCE as single solutes. Section 6.3 presents the results for the methanol slug tests in which cosolvent levels of methanol were used to displace water from the column. Section 6.4 presents the PCE breakthrough curves subject to MeOH cosolvent levels. Throughout Chapter 6, the breakthrough data are plotted along with CFITM model output derived from the curve fitting protocols discussed in Section 5.5. Output from the CFITM program for each column run is included in Appendix C, CFITM Data Output.

The breakthrough curves for each of the column runs are shown in the following sections. As discussed previously in Section 5.6, all of the breakthrough curves are similar in shape to the output curves shown in Figure 5-2.

## *6.2 Miscible Displacement Results: Methanol and PCE*

The first two sets of column experiments were tracer studies employing dilute amounts of either $^{14}C$-labeled MeOH or $^{14}C$-labeled PCE. In each case, the input pulse contained no methanol (0% methanol fraction). The purpose of the tracers was to provide a basis for comparison of the methanol displacement experiments and the PCE mobilization experiments. Figure 6-1 shows the tracer run for the $^{14}C$-labeled MeOH. Figure 6-2 shows the tracer run for the $^{14}C$-labeled PCE.

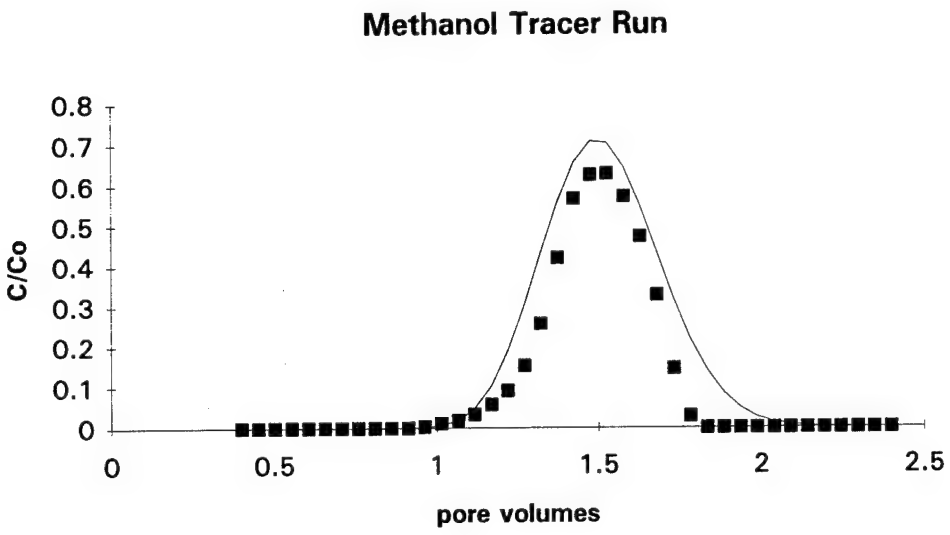


Figure 6-1. Methanol tracer breakthrough curve for a 0.745 mL/min flowrate.

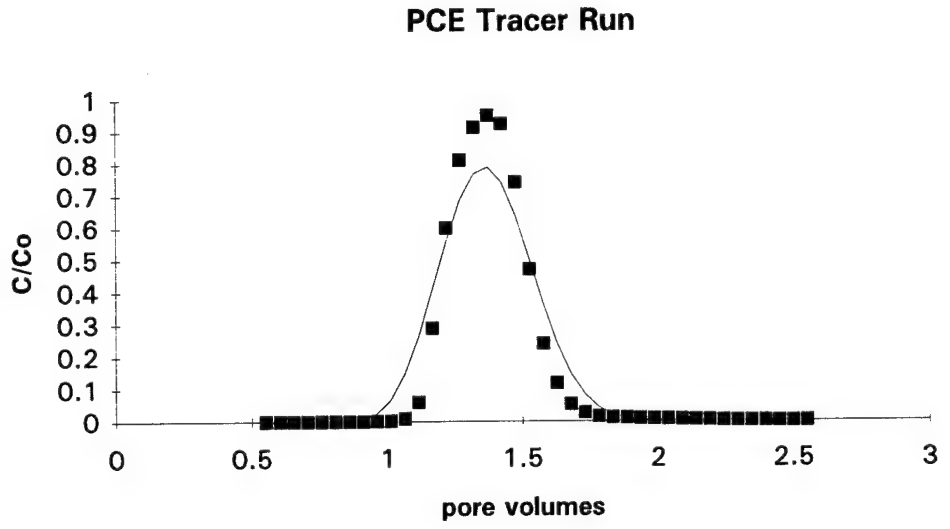


Figure 6-2. PCE tracer breakthrough curve for a 0.745 mL/min flowrate.

The solid squares on Figure 6-1 and Figure 6-2 represent the experimental data. The solid line represents CFITM's best-fitting curve, using a Peclet number equal to 159. A summary of the methanol and PCE tracer tests are shown below in Table 6-1.

| Column Run | Methanol (%) | Flow (mL/min) | Peclet Number | Retardation Factor | 95% Confidence Limit | |
|---|---|---|---|---|---|---|
| | | | | | Lower | Upper |
| Tracer MeOH | 0 | 0.745 | ***159*** | 1.00 | 112 | 206 |
| Tracer PCE | 0 | 0.745 | 159 | ***1.20*** | 1.18 | 1.22 |

Table 6-1. Summary of Methanol and PCE Tracer Runs.

Note- Numbers in bold italics indicate fitted data.

For each of the methanol tracer runs, the breakthrough curve begins to appear at approximately one pore volume. The expectation is that the center of the breakthrough curve should elute at one pore volume plus half of the total length of the input pulse (also in pore volumes). The center of the methanol tracer breakthrough curve occurs, for each tracer run, at approximately 1.5 pore volumes. The peaks arrive slightly later than expected; however, considering experimental error, the tracer curves show that the methanol was transported with the pore water, and not retarded.

The experimental tracer runs exhibited predictable behavior. The 0.745 mL/min flow rate used in each of the column runs was a relatively fast flow rate as shown by the shape of the breakthrough curves. The sharpness of the front and elution portions of the curves were indicative of advection dominated transport characteristic of a high Peclet number.

## *6.3 MeOH Displacement Experiments*

The objective of the second set of column experiments was to characterize the advection and dispersion behavior of methanol as a cosolvent. More specifically, the purpose was to characterize the extent that methanol displacing water behaved immiscibly, due to density and viscosity differences. The methanol fractions tested (1%, 5%, 10%, 20%, and 50% v/v) exhibited similar behavior. Figures 6-3 through 6-7 show the methanol breakthrough curves for the 1%, 5%, 10%, 20%, and 50% methanol fractions respectively.

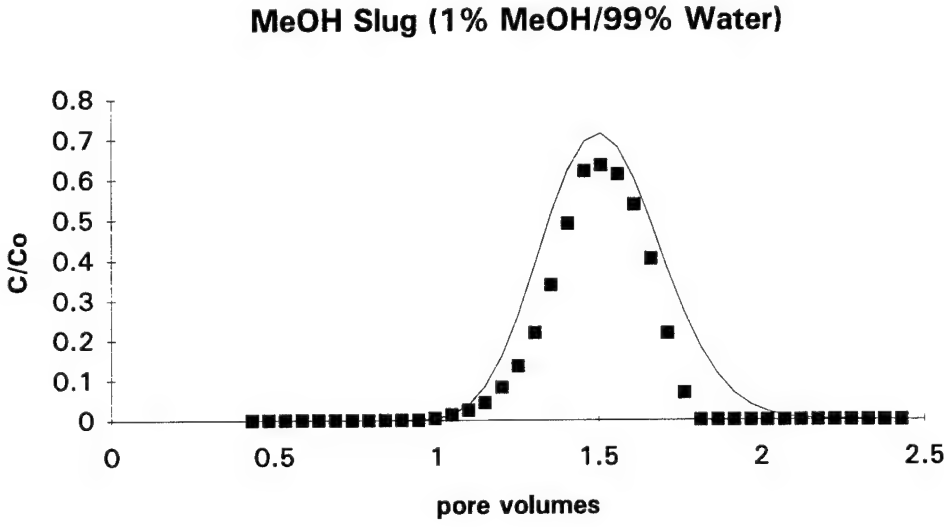


Figure 6-3. 1% MeOH slug breakthrough at a 0.745 mL/min flowrate.

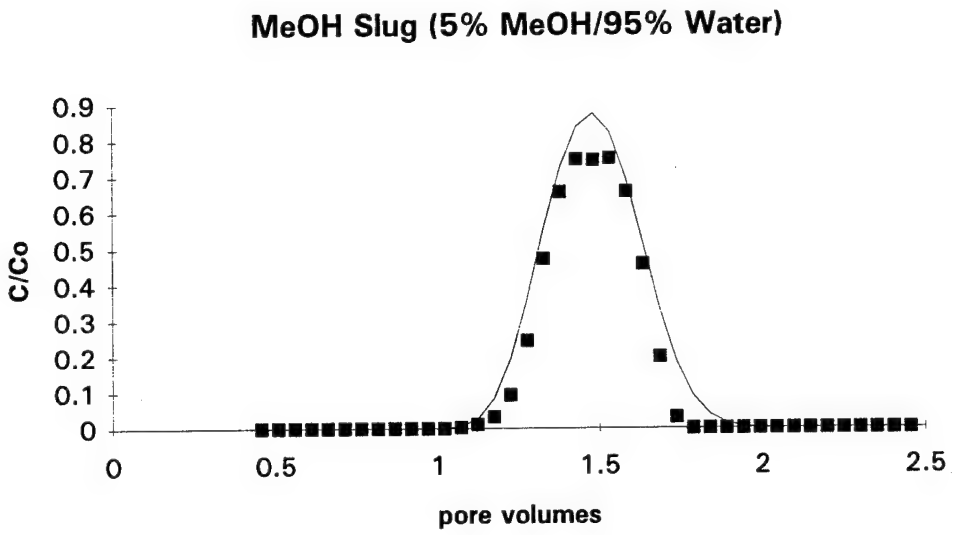


Figure 6-4. 5% MeOH slug breakthrough at a 0.745 mL/min flowrate.

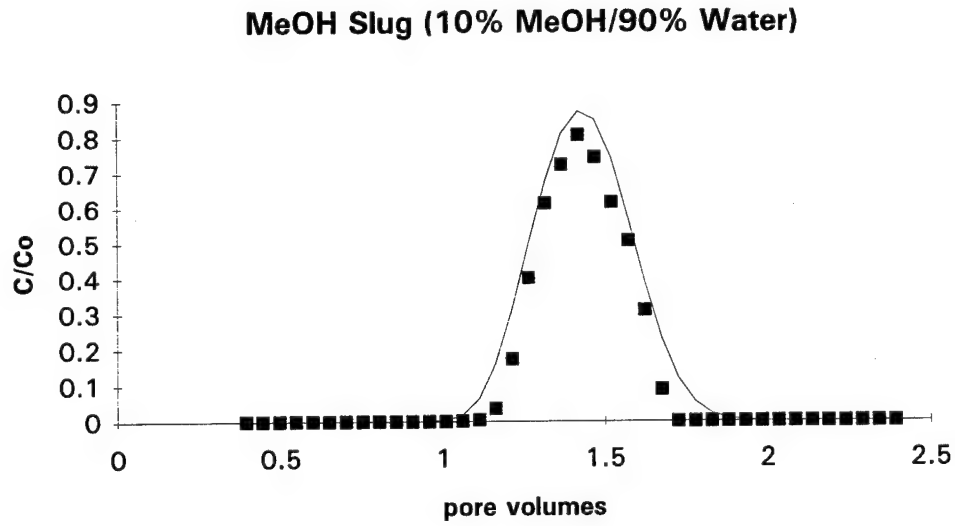


Figure 6-5. 10% MeOH slug breakthrough at a 0.745 mL/min flowrate.

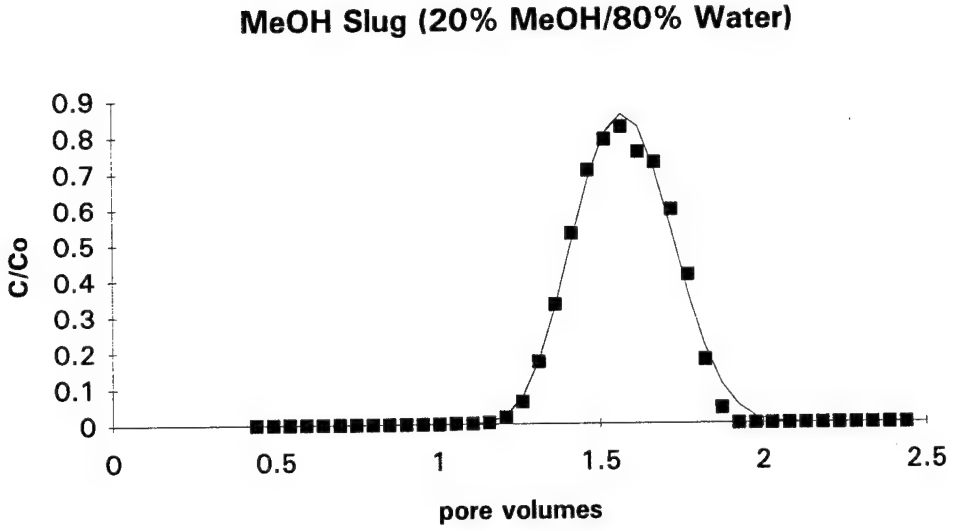


Figure 6-6. 20% MeOH slug breakthrough at a 0.745 mL/min flowrate.

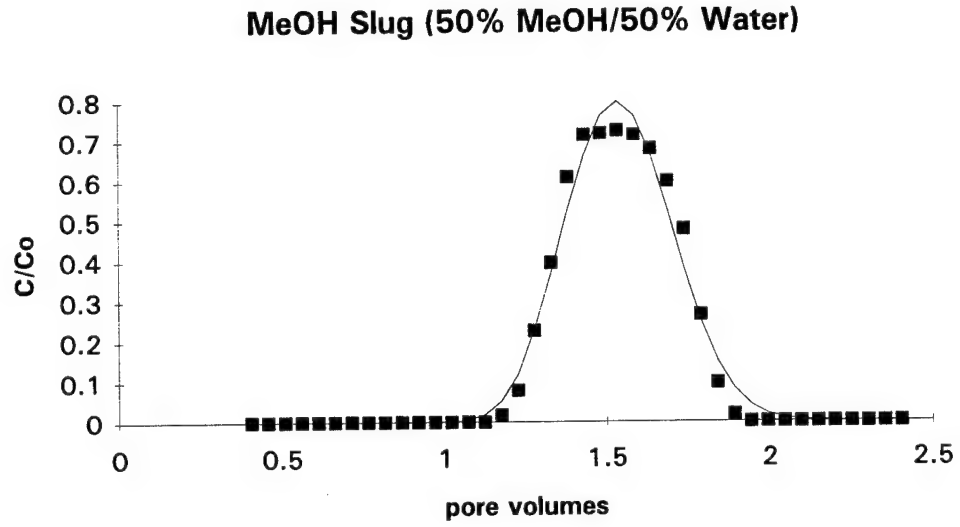


Figure 6-7. 50% MeOH slug breakthrough at a 0.745 mL/min flowrate.

The simulation providing the best-fit for the data was characterized by a Peclet number of 328, the resulting Peclet number for the 20% MeOH fraction. Each of the column runs

had similar square mass inputs (pulses). When calculating the area below each of the output curves, it was estimated that at least 93% of the mass input was conserved for each column run (Appendix A, Column Run Spreadsheets).

Each of the column runs produced breakthrough curves that were characteristic of advection dominated transport. Analysis of the breakthrough curves shows that there was no evidence of unstable fronts nor was there evidence of "over-riding" or "wedging" of methanol over water. Table 6-2 summarizes the results of the MeOH slug experiments.

| Column Run | Methanol (%) | Flow (mL/min) | Peclet Number | Retardation Factor | 95% Confidence Limit | |
|---|---|---|---|---|---|---|
| | | | | | Lower | Upper |
| MeOH Slug | 1 | 0.745 | ***153*** | 1.00 | 106 | 200 |
| MeOH Slug | 5 | 0.745 | ***305*** | 1.00 | 224 | 385 |
| MeOH Slug | 10 | 0.745 | ***276*** | 1.00 | 199 | 352 |
| MeOH Slug | 20 | 0.745 | ***328*** | 1.00 | 293 | 364 |
| MeOH Slug | 50 | 0.745 | ***221*** | 1.00 | 190 | 253 |

Table 6-2. Summary of MeOH Slug Experiments.

Note- Numbers in bold italics indicate fitted data.

The MeOH slug run at 1% methanol by volume was characterized by a Peclet number similar to that of the MeOH tracer run. However, the methanol runs with greater methanol percentages by volume were characterized by significantly larger Peclet numbers. The sharpness of the corresponding curve fronts were also indicative of the larger Peclet numbers. Each of the methanol runs exhibited early breakthrough, however,

this was due to improperly flushing the radio-labeled MeOH from the previous column experiments. An adjusted $C/C_o$ value was calculated to correct for this inaccuracy.

## *6.4 PCE Mobilization Breakthrough Curves*

The final set of experiments determined the effect of different methanol fractions on the mobilization of PCE in the soil column. Again, the methanol fractions tested (1%, 5%, 10%, 20%, and 50% v/v) exhibited similar behavior. From the output curves, one would expect that with increasing methanol fraction, the curves would exhibit earlier breakthrough, indicative of a decrease of the retardation factor of PCE. Figures 6-8 through 6-12 show the PCE mobilization breakthrough curves for each of the methanol fractions.

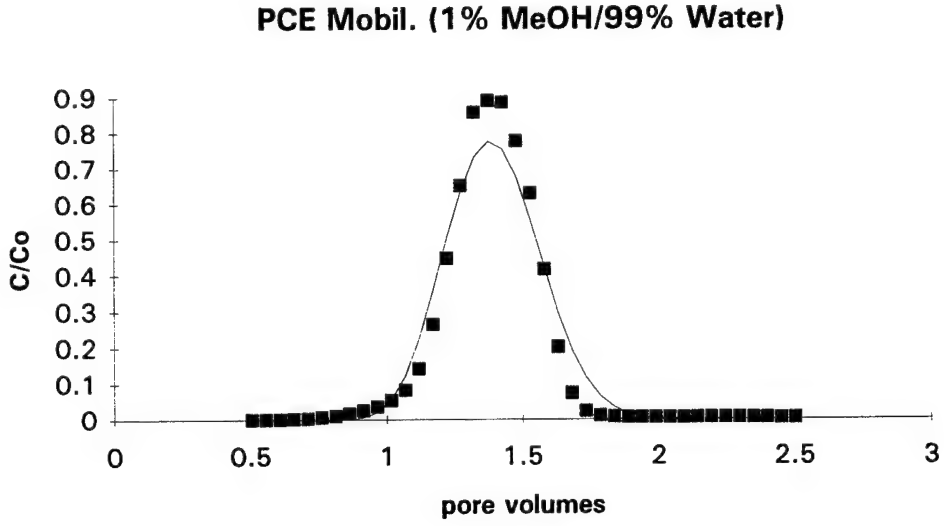


Figure 6-8. PCE mobilization breakthrough (1% MeOH) at a 0.745 mL/min flowrate.

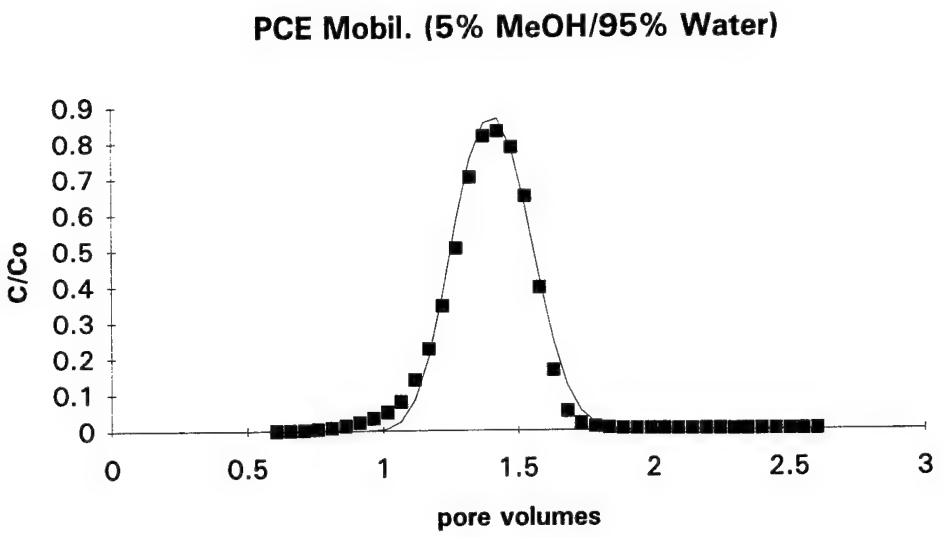


Figure 6-9. PCE mobilization breakthrough (5% MeOH) at a 0.745 mL/min flowrate.

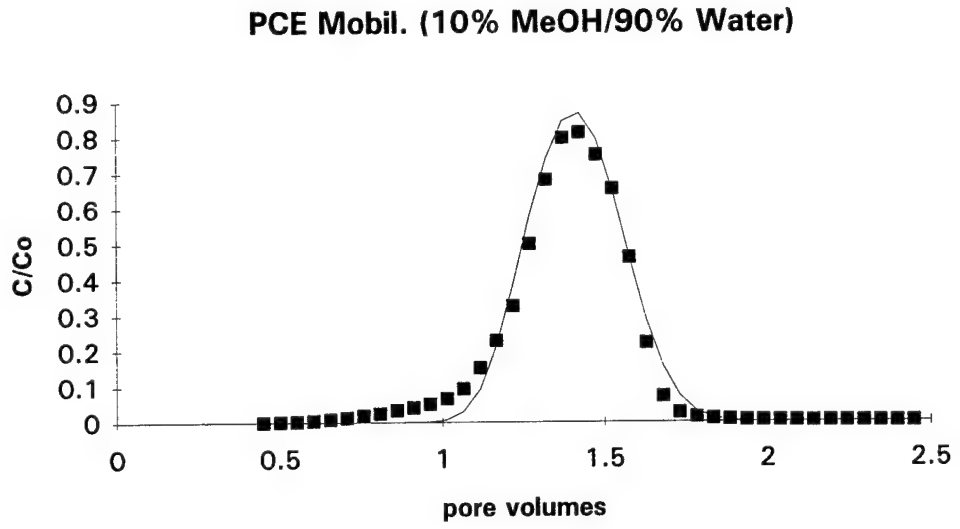


Figure 6-10. PCE mobilization breakthrough (10% MeOH) at a 0.745 mL/min flowrate.

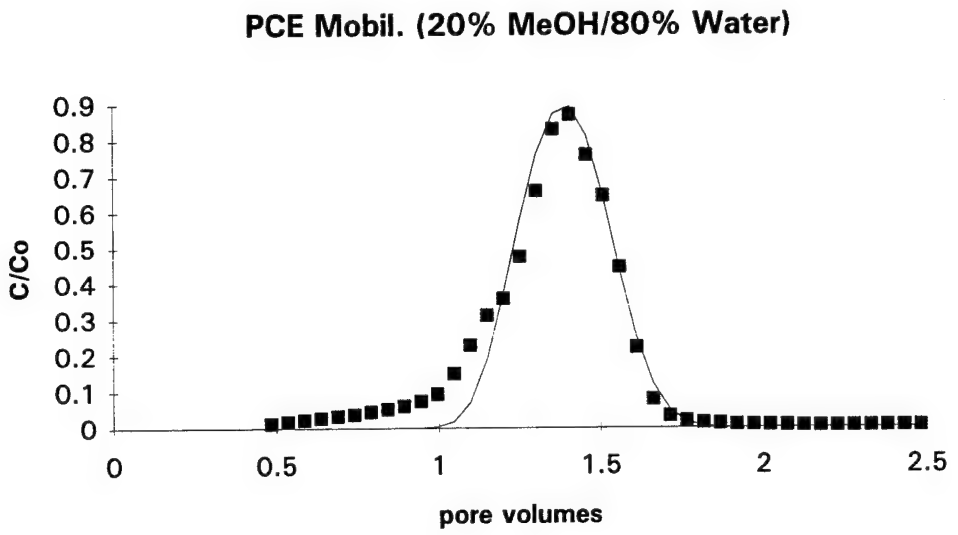


Figure 6-11. PCE mobilization breakthrough (20% MeOH) at a 0.745 mL/min flowrate.

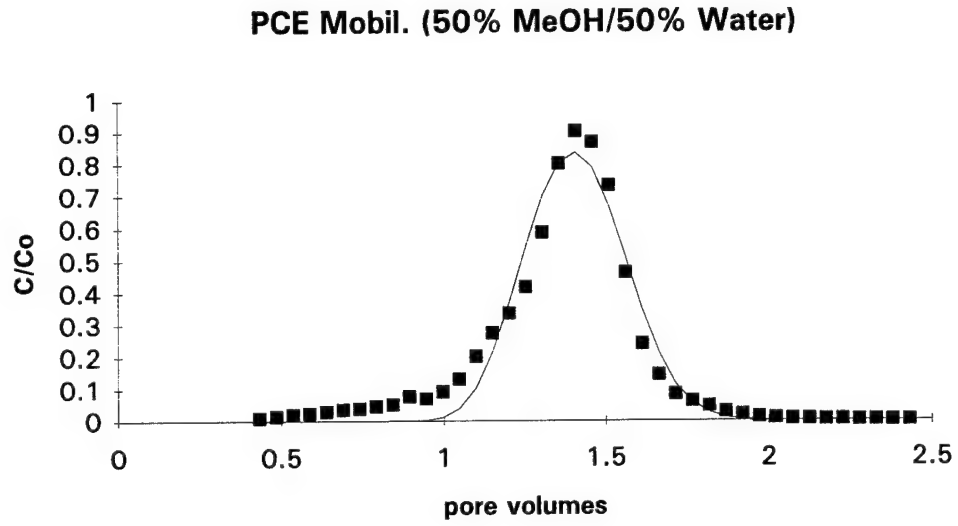


Figure 6-12. PCE mobilization breakthrough (50% MeOH) at a 0.745 mL/min flowrate.

All of the PCE retardation results (1%, 5%, 10%, 20%, and 50%) were similar. As with the MeOH slug runs, each of the PCE mobilization column runs produced breakthrough

curves that were characteristic of advection dominated transport. The simulation providing the best-fit for the data was characterized by a retardation factor of 1.22, corresponding to the 20% MeOH fraction. Each of the column runs had similar square mass inputs (pulses). When calculating the area below each of the output curves, it was estimated that at least 97% of the mass input was conserved for each column run. Table 6-3 summarizes the PCE retardation results.

| Column Run | Methanol (%) | Flow (mL/min) | Peclet Number | Retardation Factor | 95% Confidence Limit | |
|---|---|---|---|---|---|---|
| | | | | | Lower | Upper |
| PCE Input | 1 | 0.745 | 153 | ***1.22*** | 1.21 | 1.24 |
| PCE Input | 5 | 0.745 | 305 | ***1.25*** | 1.25 | 1.26 |
| PCE Input | 10 | 0.745 | 276 | ***1.25*** | 1.24 | 1.26 |
| PCE Input | 20 | 0.745 | 328 | ***1.23*** | 1.22 | 1.24 |
| PCE Input | 50 | 0.745 | 221 | ***1.24*** | 1.23 | 1.25 |

Table 6-3. Summary of PCE Retardation Experiments.

Note- Numbers in bold italics indicate fitted data.

In general, the PCE breakthrough curves were symmetrical and weakly retarded. The PCE runs with 20% methanol and 50% methanol each exhibited slightly early breakthrough and slight tailing.

Van Genuchten's Least Squares Program determined the best-fitting retardation factor for each of the observed breakthrough curves. All of the resulting retardation factors are plotted in Figure 6-13 as a function of the methanol fraction.

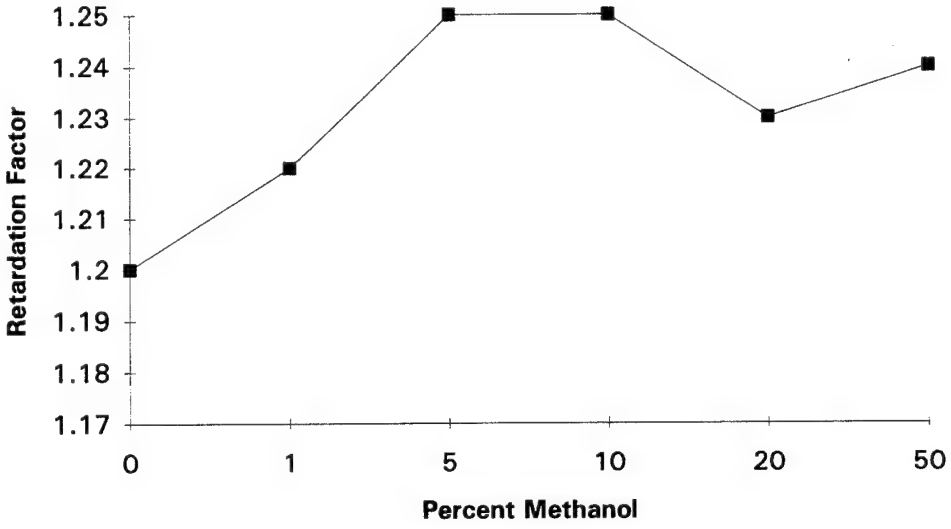


Figure 6-13. Retardation Factors with respect to methanol fractions.

The results do not indicate any trends. The retardation factor only varied between 1.20 and 1.25. Essentially, there was no significant difference in retardation factor with increasing methanol fraction.

The PCE mobilization experiments failed to demonstrate the hypothesized results. The degree of retardation of PCE did not decrease log-linearly with increasing methanol fraction. However, the results of this study confirmed the results of previous studies (Imhoff, 1995). The MeOH slug experiments showed that with an increasing methanol fraction, there was an increase in the Peclet number.

# *Chapter 7. Summary and Conclusions*

The goal of this research was to test the ability of methanol as an effective cosolvent. This study investigated the transport and dissolution of methanol in a water-saturated porous medium and the effects of methanol on the mobilization of PCE. 1-D column experiments were used to examine: the transport behavior of trace amounts of $^{14}C$-labeled methanol/PCE in water; the transport of various methanol fractions through a sand column; and, methanol mobilizing PCE in a saturated soil column.

The one-dimensional column apparatus devised for this work performed adequately. An average of 95% of the mass input through the column was calculated in the mass output indicating that a majority of the mass was conserved. The tracer and slug breakthrough curves of the methanol were described well by the advection/dispersion equation, and showed no indications of density and viscosity difference effects.

For the 1-D laboratory column at the flowrate tested (0.745 mL/min), methanol failed to produce the hypothesized cosolvent effect in mobilizing PCE. Two possible reasons for this failure exist: (1) The PCE sorbed too weakly to the porous medium and any reductions in the sorption were difficult to observe given the experimental uncertainty produced by the methods; (2) The MeOH front by-passed much of the porous medium, thereby failing to mix sufficiently in a timely manner. Given the apparent stability of the methanol slug breakthrough curves, the first reason appears to be the more likely of the two.

Further studies on flow conditions in a contaminated region need to be investigated. Perhaps the 0.745 mL/min flow rate used in this study was too fast to adequately demonstrate the impact of methanol on sorption rates. Although the outcome of this research was not completely as expected, the results do provide motivation for future work to address these flow and transport issues.

# *Appendix A. Column Run Spreadsheets*

*Explanation of Terms for Spreadsheets-*

**__/__%**: Type of column run. First number refers to MeOH fraction; second number refers to percent water.

**flow**: flow rate at which the experiment was conducted.

**time**: the time at which the sample was completed. For each of the column runs, the sample time in the vial was 20 seconds, the wash time in the waste stream was 100 seconds, and the time in between sampling and washing was 3 seconds. Total time between sampling vials was 123 seconds (2 minutes, 3 seconds).

**conv.**: time conversion to decimals.

**pore vol.**: time conversion to equivalent, unitless "pore volumes."

**dpm**: "disintegrations per minute" as recorded by the scintillation counter. (dpm = concentration [C]).

**diff**: Difference in weight [g] between the sample vial initially and the sample vial after sampling.

**dpm/diff**: Self-explanatory. Assuming the density of water is 1 g per $cm^3$, [dpm/mL].

**Co**: Initial concentration of input pulse [dpm/mL].

**C/Co**: Dimensionless parameter [sample concentration/initial concentration].

**Adj C/Co**: Adjusted C/Co value to account for inaccuracies caused by insufficient column flushing [-].

**M**: Mass of radio-labeled MeOH or PCE in the sample vial [dpm].

**Mo**: Initial mass of input pulse [dpm].

**M/Mo**: Dimensionless parameter [sample mass/total initial mass].

**CFIT**: Fitted value by van Genuchten's model based on experimental output [dpm/mL].

| 0/100% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:16:00 | 16 | 0.4 | 2352.17 | 0.28218 | 8335.708 | 184149.3 | 0.045266 | -0.00473 | 12730.71 | 1749188 | 0.007278 | | 0.4 | 0 |
| tracer | 0:18:03 | 18.05 | 0.45125 | 2741.78 | 0.27514 | 9965.036 | 184149.3 | 0.054114 | 0.004114 | 15219.1 | 1749188 | 0.008701 | | 0.45125 | 0 |
| | 0:20:06 | 20.1 | 0.5025 | 3187.25 | 0.29624 | 10759.01 | 184149.3 | 0.058425 | 0.008425 | 16431.7 | 1749188 | 0.009394 | | 0.5025 | 0 |
| flow | 0:22:09 | 22.15 | 0.55375 | 2707.42 | 0.2523 | 10730.96 | 184149.3 | 0.058273 | 0.008273 | 16388.85 | 1749188 | 0.009369 | | 0.55375 | 0 |
| 0.745 | 0:24:12 | 24.2 | 0.605 | 3007.02 | 0.2978 | 10097.45 | 184149.3 | 0.054833 | 0.004833 | 15421.33 | 1749188 | 0.008816 | | 0.605 | 0 |
| (mL/min) | 0:26:15 | 26.25 | 0.65625 | 2692.45 | 0.28399 | 9480.792 | 184149.3 | 0.051484 | 0.001484 | 14479.54 | 1749188 | 0.008278 | | 0.65625 | 0 |
| | 0:28:18 | 28.3 | 0.7075 | 2700.31 | 0.29565 | 9133.469 | 184149.3 | 0.049598 | -0.0004 | 13949.09 | 1749188 | 0.007975 | | 0.7075 | 0 |
| | 0:30:21 | 30.35 | 0.75875 | 2422.26 | 0.26239 | 9231.526 | 184149.3 | 0.050131 | 0.000131 | 14098.85 | 1749188 | 0.00806 | | 0.75875 | 0 |
| | 0:32:24 | 32.4 | 0.81 | 2654.62 | 0.29869 | 8887.542 | 184149.3 | 0.048263 | -0.00174 | 13573.5 | 1749188 | 0.00776 | | 0.81 | 0 |
| | 0:34:27 | 34.45 | 0.86125 | 2475.85 | 0.28079 | 8817.444 | 184149.3 | 0.047882 | -0.00212 | 13466.44 | 1749188 | 0.007699 | | 0.86125 | 0 |
| | 0:36:30 | 36.5 | 0.9125 | 2729.84 | 0.30155 | 9052.694 | 184149.3 | 0.04916 | -0.00084 | 13825.73 | 1749188 | 0.007904 | | 0.9125 | 0 |
| | 0:38:33 | 38.55 | 0.96375 | 2834.39 | 0.29127 | 9731.143 | 184149.3 | 0.052844 | 0.002844 | 14861.89 | 1749188 | 0.008496 | | 0.96375 | 0.001 |
| | 0:40:36 | 40.6 | 1.015 | 3256.88 | 0.28962 | 11245.36 | 184149.3 | 0.061067 | 0.011067 | 17174.47 | 1749188 | 0.009819 | | 1.015 | 0.006 |
| | 0:42:39 | 42.65 | 1.06625 | 3524.05 | 0.27962 | 12603 | 184149.3 | 0.068439 | 0.018439 | 19247.93 | 1749188 | 0.011004 | | 1.06625 | 0.018 |
| | 0:44:42 | 44.7 | 1.1175 | 4402.99 | 0.29154 | 15102.52 | 184149.3 | 0.082012 | 0.032012 | 23065.33 | 1749188 | 0.013186 | | 1.1175 | 0.048 |
| | 0:46:45 | 46.75 | 1.16875 | 5379.17 | 0.27474 | 19579.13 | 184149.3 | 0.106322 | 0.056322 | 29902.23 | 1749188 | 0.017095 | | 1.16875 | 0.103 |
| | 0:48:48 | 48.8 | 1.22 | 6793.25 | 0.26143 | 25984.97 | 184149.3 | 0.141108 | 0.091108 | 39685.54 | 1749188 | 0.022688 | | 1.22 | 0.189 |
| | 0:50:51 | 50.85 | 1.27125 | 10285.85 | 0.2756 | 37321.66 | 184149.3 | 0.202671 | 0.152671 | 56999.51 | 1749188 | 0.032586 | | 1.27125 | 0.303 |
| | 0:52:54 | 52.9 | 1.3225 | 16182.19 | 0.28659 | 56464.6 | 184149.3 | 0.306624 | 0.256624 | 86235.56 | 1749188 | 0.0493 | | 1.3225 | 0.434 |
| | 0:54:57 | 54.95 | 1.37375 | 22785.14 | 0.263 | 86635.51 | 184149.3 | 0.470463 | 0.420463 | 132314.1 | 1749188 | 0.075643 | | 1.37375 | 0.558 |
| | 0:57:00 | 57 | 1.425 | 32800.14 | 0.28845 | 113711.7 | 184149.3 | 0.617497 | 0.567497 | 173666.2 | 1749188 | 0.099284 | | 1.425 | 0.656 |
| | 0:59:03 | 59.05 | 1.47625 | 35488.19 | 0.2851 | 124476.3 | 184149.3 | 0.675953 | 0.625953 | 190106.4 | 1749188 | 0.108683 | | 1.47625 | 0.708 |
| | 1:01:06 | 61.1 | 1.5275 | 33544.8 | 0.26831 | 125022.5 | 184149.3 | 0.678919 | 0.628919 | 190940.7 | 1749188 | 0.10916 | | 1.5275 | 0.704 |
| | 1:03:09 | 63.15 | 1.57875 | 32803.06 | 0.28581 | 114772.3 | 184149.3 | 0.623256 | 0.573256 | 175285.9 | 1749188 | 0.10021 | | 1.57875 | 0.646 |
| | 1:05:12 | 65.2 | 1.63 | 28218.48 | 0.29288 | 96348.27 | 184149.3 | 0.523207 | 0.473207 | 147147.9 | 1749188 | 0.084124 | | 1.63 | 0.55 |
| | 1:07:15 | 67.25 | 1.68125 | 19814.25 | 0.28503 | 69516.37 | 184149.3 | 0.3775 | 0.3275 | 106168.9 | 1749188 | 0.060696 | | 1.68125 | 0.435 |
| | 1:09:18 | 69.3 | 1.7325 | 10091.8 | 0.28028 | 36006.14 | 184149.3 | 0.195527 | 0.145527 | 54990.37 | 1749188 | 0.031438 | | 1.7325 | 0.318 |
| | 1:11:21 | 71.35 | 1.78375 | 4031.68 | 0.27924 | 14438.05 | 184149.3 | 0.078404 | 0.028404 | 22050.51 | 1749188 | 0.012606 | | 1.78375 | 0.219 |
| | 1:13:24 | 73.4 | 1.835 | 1401.85 | 0.26025 | 5386.551 | 184149.3 | 0.029251 | -0.02075 | 8226.611 | 1749188 | 0.004703 | | 1.835 | 0.141 |
| | 1:15:27 | 75.45 | 1.88625 | 730.66 | 0.28264 | 2585.126 | 184149.3 | 0.014038 | -0.03596 | 3948.134 | 1749188 | 0.002257 | | 1.88625 | 0.086 |
| | 1:17:30 | 77.5 | 1.9375 | 562.14 | 0.28621 | 1964.082 | 184149.3 | 0.010666 | -0.03933 | 2999.645 | 1749188 | 0.001715 | | 1.9375 | 0.049 |
| | 1:19:33 | 79.55 | 1.98875 | 433.23 | 0.25932 | 1670.639 | 184149.3 | 0.009072 | -0.04093 | 2551.483 | 1749188 | 0.001459 | | 1.98875 | 0.026 |
| | 1:21:36 | 81.6 | 2.04 | 435.98 | 0.28769 | 1515.451 | 184149.3 | 0.008229 | -0.04177 | 2314.472 | 1749188 | 0.001323 | | 2.04 | 0.014 |
| | 1:23:39 | 83.65 | 2.09125 | 377.34 | 0.2784 | 1355.388 | 184149.3 | 0.00736 | -0.04264 | 2070.016 | 1749188 | 0.001183 | | 2.09125 | 0.007 |
| | 1:25:42 | 85.7 | 2.1425 | 352.89 | 0.28682 | 1230.354 | 184149.3 | 0.006681 | -0.04332 | 1879.057 | 1749188 | 0.001074 | | 2.1425 | 0.003 |
| | 1:27:45 | 87.75 | 2.19375 | 309.22 | 0.29346 | 1053.704 | 184149.3 | 0.005722 | -0.04428 | 1609.27 | 1749188 | 0.00092 | | 2.19375 | 0.001 |
| | 1:29:48 | 89.8 | 2.245 | 269.96 | 0.2791 | 967.2519 | 184149.3 | 0.005253 | -0.04475 | 1477.235 | 1749188 | 0.000845 | | 2.245 | 0.001 |
| | 1:31:51 | 91.85 | 2.29625 | 241.06 | 0.27528 | 875.6902 | 184149.3 | 0.004755 | -0.04524 | 1337.398 | 1749188 | 0.000765 | | 2.29625 | 0 |
| | 1:33:54 | 93.9 | 2.3475 | 224.67 | 0.29142 | 770.9491 | 184149.3 | 0.004187 | -0.04581 | 1177.432 | 1749188 | 0.000673 | | 2.3475 | 0 |
| | 1:35:57 | 95.95 | 2.39875 | 209.46 | 0.29172 | 718.0173 | 184149.3 | 0.003899 | -0.0461 | 1096.592 | 1749188 | 0.000627 | | 2.39875 | 0 |
| | | | | | | | | | | 1670116 | | 0.954795 | | | |

| 1/99% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:17:15 | 17.25 | 0.43125 | 3121.88 | 0.27801 | 11229.38 | 230856 | 0.048642 | -0.00136 | 17150.07 | 2235840 | 0.007671 | | 0.43125 | 0 |
| slug | 0:19:18 | 19.3 | 0.4825 | 3674.83 | 0.28193 | 13034.55 | 230856 | 0.056462 | 0.006462 | 19907.01 | 2235840 | 0.008904 | | 0.4825 | 0 |
| | 0:21:21 | 21.35 | 0.53375 | 3697.04 | 0.2748 | 13453.57 | 230856 | 0.058277 | 0.008277 | 20546.96 | 2235840 | 0.00919 | | 0.53375 | 0 |
| flow | 0:23:24 | 23.4 | 0.585 | 3796.5 | 0.30203 | 12569.94 | 230856 | 0.054449 | 0.004449 | 19197.45 | 2235840 | 0.008586 | | 0.585 | 0 |
| 0.745 | 0:25:27 | 25.45 | 0.63625 | 3512.64 | 0.28971 | 12124.68 | 230856 | 0.052521 | 0.002521 | 18517.41 | 2235840 | 0.008282 | | 0.63625 | 0 |
| (mL/min) | 0:27:30 | 27.5 | 0.6875 | 3261.61 | 0.2771 | 11770.52 | 230856 | 0.050986 | 0.000986 | 17976.52 | 2235840 | 0.00804 | | 0.6875 | 0 |
| | 0:29:33 | 29.55 | 0.73875 | 3053.51 | 0.27453 | 11122.68 | 230856 | 0.04818 | -0.00182 | 16987.12 | 2235840 | 0.007598 | | 0.73875 | 0 |
| | 0:31:36 | 31.6 | 0.79 | 3170.53 | 0.29584 | 10717.04 | 230856 | 0.046423 | -0.00358 | 16367.6 | 2235840 | 0.007321 | | 0.79 | 0 |
| | 0:33:39 | 33.65 | 0.84125 | 3199.38 | 0.30043 | 10649.34 | 230856 | 0.04613 | -0.00387 | 16264.2 | 2235840 | 0.007274 | | 0.84125 | 0 |
| | 0:35:42 | 35.7 | 0.8925 | 3206.62 | 0.29939 | 10710.51 | 230856 | 0.046395 | -0.00361 | 16357.63 | 2235840 | 0.007316 | | 0.8925 | 0 |
| | 0:37:45 | 37.75 | 0.94375 | 3601.85 | 0.31185 | 11549.94 | 230856 | 0.050031 | 3.09E-05 | 17639.65 | 2235840 | 0.007889 | | 0.94375 | 0.001 |
| | 0:39:48 | 39.8 | 0.995 | 3707.97 | 0.29429 | 12599.71 | 230856 | 0.054578 | 0.004578 | 19242.91 | 2235840 | 0.008607 | | 0.995 | 0.004 |
| | 0:41:51 | 41.85 | 1.04625 | 3972.68 | 0.27078 | 14671.25 | 230856 | 0.063552 | 0.013552 | 22406.66 | 2235840 | 0.010022 | | 1.04625 | 0.014 |
| | 0:43:54 | 43.9 | 1.0975 | 5170.31 | 0.30059 | 17200.54 | 230856 | 0.074508 | 0.024508 | 26269.52 | 2235840 | 0.011749 | | 1.0975 | 0.037 |
| | 0:45:57 | 45.95 | 1.14875 | 6813.97 | 0.31523 | 21615.87 | 230856 | 0.093634 | 0.043634 | 33012.83 | 2235840 | 0.014765 | | 1.14875 | 0.084 |
| | 0:48:00 | 48 | 1.2 | 9274.81 | 0.30432 | 30477.16 | 230856 | 0.132018 | 0.082018 | 46546.25 | 2235840 | 0.020818 | | 1.2 | 0.159 |
| | 0:50:03 | 50.05 | 1.25125 | 10656.11 | 0.24923 | 42756.13 | 230856 | 0.185207 | 0.135207 | 65299.3 | 2235840 | 0.029206 | | 1.25125 | 0.262 |
| | 0:52:06 | 52.1 | 1.3025 | 18798.31 | 0.30392 | 61852.82 | 230856 | 0.267928 | 0.217928 | 94464.72 | 2235840 | 0.04225 | | 1.3025 | 0.388 |
| | 0:54:09 | 54.15 | 1.35375 | 25062.83 | 0.27956 | 89650.99 | 230856 | 0.388342 | 0.338342 | 136919.5 | 2235840 | 0.061238 | | 1.35375 | 0.515 |
| | 0:56:12 | 56.2 | 1.405 | 36976.07 | 0.2969 | 124540.5 | 230856 | 0.539473 | 0.489473 | 190204.5 | 2235840 | 0.085071 | | 1.405 | 0.623 |
| | 0:58:15 | 58.25 | 1.45625 | 45216.18 | 0.2926 | 154532.4 | 230856 | 0.669389 | 0.619389 | 236009.6 | 2235840 | 0.105557 | | 1.45625 | 0.694 |
| | 1:00:18 | 60.3 | 1.5075 | 43849.62 | 0.27775 | 157874.4 | 230856 | 0.683865 | 0.633865 | 241113.7 | 2235840 | 0.10784 | | 1.5075 | 0.714 |
| | 1:02:21 | 62.35 | 1.55875 | 43856.55 | 0.28728 | 152661.3 | 230856 | 0.661284 | 0.611284 | 233152 | 2235840 | 0.104279 | | 1.55875 | 0.68 |
| | 1:04:24 | 64.4 | 1.61 | 39251.06 | 0.28994 | 135376.5 | 230856 | 0.586411 | 0.536411 | 206753.7 | 2235840 | 0.092472 | | 1.61 | 0.601 |
| | 1:06:27 | 66.45 | 1.66125 | 29087.4 | 0.27819 | 104559.5 | 230856 | 0.452921 | 0.402921 | 159688.5 | 2235840 | 0.071422 | | 1.66125 | 0.494 |
| | 1:08:30 | 68.5 | 1.7125 | 20156.22 | 0.328 | 61451.89 | 230856 | 0.266191 | 0.216191 | 93852.4 | 2235840 | 0.041976 | | 1.7125 | 0.377 |
| | 1:10:33 | 70.55 | 1.76375 | 8548.3 | 0.31434 | 27194.44 | 230856 | 0.117798 | 0.067798 | 41532.71 | 2235840 | 0.018576 | | 1.76375 | 0.27 |
| | 1:12:36 | 72.6 | 1.815 | 2656.38 | 0.28023 | 9479.285 | 230856 | 0.041061 | -0.00894 | 14477.24 | 2235840 | 0.006475 | | 1.815 | 0.182 |
| | 1:14:39 | 74.65 | 1.86625 | 1208.53 | 0.31282 | 3863.34 | 230856 | 0.016735 | -0.03327 | 5900.286 | 2235840 | 0.002639 | | 1.86625 | 0.115 |
| | 1:16:42 | 76.7 | 1.9175 | 698.21 | 0.28843 | 2420.726 | 230856 | 0.010486 | -0.03951 | 3697.054 | 2235840 | 0.001654 | | 1.9175 | 0.068 |
| | 1:18:45 | 78.75 | 1.96875 | 562.67 | 0.29034 | 1937.969 | 230856 | 0.008395 | -0.04161 | 2959.764 | 2235840 | 0.001324 | | 1.96875 | 0.039 |
| | 1:20:48 | 80.8 | 2.02 | 461.87 | 0.28363 | 1628.424 | 230856 | 0.007054 | -0.04295 | 2487.011 | 2235840 | 0.001112 | | 2.02 | 0.021 |
| | 1:22:51 | 82.85 | 2.07125 | 393.61 | 0.29187 | 1348.58 | 230856 | 0.005842 | -0.04416 | 2059.619 | 2235840 | 0.000921 | | 2.07125 | 0.011 |
| | 1:24:54 | 84.9 | 2.1225 | 350.33 | 0.28569 | 1226.259 | 230856 | 0.005312 | -0.04469 | 1872.804 | 2235840 | 0.000838 | | 2.1225 | 0.005 |
| | 1:26:57 | 86.95 | 2.17375 | 304.98 | 0.27928 | 1092.022 | 230856 | 0.00473 | -0.04527 | 1667.791 | 2235840 | 0.000746 | | 2.17375 | 0.003 |
| | 1:29:00 | 89 | 2.225 | 292.26 | 0.29769 | 981.7595 | 230856 | 0.004253 | -0.04575 | 1499.392 | 2235840 | 0.000671 | | 2.225 | 0.001 |
| | 1:31:03 | 91.05 | 2.27625 | 256.34 | 0.29741 | 861.9078 | 230856 | 0.003734 | -0.04627 | 1316.349 | 2235840 | 0.000589 | | 2.27625 | 0.001 |
| | 1:33:06 | 93.1 | 2.3275 | 235.52 | 0.30255 | 778.4498 | 230856 | 0.003372 | -0.04663 | 1188.888 | 2235840 | 0.000532 | | 2.3275 | 0 |
| | 1:35:09 | 95.15 | 2.37875 | 205.92 | 0.3034 | 678.708 | 230856 | 0.00294 | -0.04706 | 1036.557 | 2235840 | 0.000464 | | 2.37875 | 0 |
| | 1:37:12 | 97.2 | 2.43 | 180.13 | 0.29762 | 605.2349 | 230856 | 0.002622 | -0.04738 | 924.3449 | 2235840 | 0.000413 | | 2.43 | 0 |
| | | | | | | | | | | | | | | | |
| | | | | | | | | | | 2084467 | | 0.932297 | | | |

| 5/95% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:18:15 | 18.25 | 0.45625 | 1961.66 | 0.30121 | 6512.599 | 207208 | 0.03143 | -0.01857 | 9946.367 | 2006809 | 0.004956 | | 0.45625 | 0 |
| slug | 0:20:18 | 20.3 | 0.5075 | 2380.78 | 0.28853 | 8251.412 | 207208 | 0.039822 | -0.01018 | 12601.97 | 2006809 | 0.00628 | | 0.5075 | 0 |
| | 0:22:21 | 22.35 | 0.55875 | 2780.3 | 0.27834 | 9988.863 | 207208 | 0.048207 | -0.00179 | 15255.49 | 2006809 | 0.007602 | | 0.55875 | 0 |
| flow | 0:24:24 | 24.4 | 0.61 | 3477.41 | 0.31543 | 11024.35 | 207208 | 0.053204 | 0.003204 | 16836.94 | 2006809 | 0.00839 | | 0.61 | 0 |
| 0.745 | 0:26:27 | 26.45 | 0.66125 | 3114.01 | 0.27814 | 11195.84 | 207208 | 0.054032 | 0.004032 | 17098.84 | 2006809 | 0.00852 | | 0.66125 | 0 |
| (mL/min) | 0:28:30 | 28.5 | 0.7125 | 2973.95 | 0.29027 | 10245.46 | 207208 | 0.049445 | -0.00055 | 15647.38 | 2006809 | 0.007797 | | 0.7125 | 0 |
| | 0:30:33 | 30.55 | 0.76375 | 2790.12 | 0.28472 | 9799.522 | 207208 | 0.047293 | -0.00271 | 14966.32 | 2006809 | 0.007458 | | 0.76375 | 0 |
| | 0:32:36 | 32.6 | 0.815 | 2642.07 | 0.27815 | 9498.724 | 207208 | 0.045841 | -0.00416 | 14506.93 | 2006809 | 0.007229 | | 0.815 | 0 |
| | 0:34:39 | 34.65 | 0.86625 | 2820 | 0.29924 | 9423.874 | 207208 | 0.04548 | -0.00452 | 14392.61 | 2006809 | 0.007172 | | 0.86625 | 0 |
| | 0:36:42 | 36.7 | 0.9175 | 2661.3 | 0.28134 | 9459.373 | 207208 | 0.045652 | -0.00435 | 14446.83 | 2006809 | 0.007199 | | 0.9175 | 0 |
| | 0:38:45 | 38.75 | 0.96875 | 2632.9 | 0.28206 | 9334.539 | 207208 | 0.045049 | -0.00495 | 14256.17 | 2006809 | 0.007104 | | 0.96875 | 0 |
| | 0:40:48 | 40.8 | 1.02 | 2643.93 | 0.26972 | 9802.499 | 207208 | 0.047308 | -0.00269 | 14970.87 | 2006809 | 0.00746 | | 1.02 | 0.001 |
| | 0:42:51 | 42.85 | 1.07125 | 2955.27 | 0.2723 | 10852.99 | 207208 | 0.052377 | 0.002377 | 16575.23 | 2006809 | 0.008259 | | 1.07125 | 0.006 |
| | 0:44:54 | 44.9 | 1.1225 | 3352.62 | 0.26606 | 12600.99 | 207208 | 0.060813 | 0.010813 | 19244.87 | 2006809 | 0.00959 | | 1.1225 | 0.026 |
| | 0:46:57 | 46.95 | 1.17375 | 5125.82 | 0.30247 | 16946.54 | 207208 | 0.081785 | 0.031785 | 25881.6 | 2006809 | 0.012897 | | 1.17375 | 0.083 |
| | 0:49:00 | 49 | 1.225 | 8279.97 | 0.28032 | 29537.56 | 207208 | 0.14255 | 0.09255 | 45111.24 | 2006809 | 0.022479 | | 1.225 | 0.194 |
| | 0:51:03 | 51.05 | 1.27625 | 16937.52 | 0.27741 | 61055.91 | 207208 | 0.29466 | 0.24466 | 93247.64 | 2006809 | 0.046466 | | 1.27625 | 0.36 |
| | 0:53:06 | 53.1 | 1.3275 | 30171.24 | 0.27897 | 108152.3 | 207208 | 0.52195 | 0.47195 | 165175.6 | 2006809 | 0.082308 | | 1.3275 | 0.554 |
| | 0:55:09 | 55.15 | 1.37875 | 41412.09 | 0.28258 | 146550 | 207208 | 0.70726 | 0.65726 | 223818.4 | 2006809 | 0.111529 | | 1.37875 | 0.724 |
| | 0:57:12 | 57.2 | 1.43 | 45529.53 | 0.27524 | 165417.6 | 207208 | 0.798316 | 0.748316 | 252634 | 2006809 | 0.125888 | | 1.43 | 0.838 |
| | 0:59:15 | 59.25 | 1.48125 | 44188.59 | 0.26808 | 164833.6 | 207208 | 0.795498 | 0.745498 | 251742.1 | 2006809 | 0.125444 | | 1.48125 | 0.875 |
| | 1:01:18 | 61.3 | 1.5325 | 45227.63 | 0.2725 | 165973 | 207208 | 0.800997 | 0.750997 | 253482.2 | 2006809 | 0.126311 | | 1.5325 | 0.824 |
| | 1:03:21 | 63.35 | 1.58375 | 39982.63 | 0.27252 | 146714.5 | 207208 | 0.708054 | 0.658054 | 224069.7 | 2006809 | 0.111655 | | 1.58375 | 0.693 |
| | 1:05:24 | 65.4 | 1.635 | 30932.71 | 0.29456 | 105013.3 | 207208 | 0.506801 | 0.456801 | 160381.5 | 2006809 | 0.079919 | | 1.635 | 0.513 |
| | 1:07:27 | 67.45 | 1.68625 | 13818.47 | 0.26754 | 51650.11 | 207208 | 0.249267 | 0.199267 | 78882.63 | 2006809 | 0.039307 | | 1.68625 | 0.332 |
| | 1:09:30 | 69.5 | 1.7375 | 4242.49 | 0.2554 | 16611.16 | 207208 | 0.080167 | 0.030167 | 25369.39 | 2006809 | 0.012642 | | 1.7375 | 0.185 |
| | 1:11:33 | 71.55 | 1.78875 | 1582.39 | 0.30033 | 5268.838 | 207208 | 0.025428 | -0.02457 | 8046.832 | 2006809 | 0.00401 | | 1.78875 | 0.091 |
| | 1:13:36 | 73.6 | 1.84 | 785.96 | 0.28855 | 2723.826 | 207208 | 0.013145 | -0.03685 | 4159.963 | 2006809 | 0.002073 | | 1.84 | 0.039 |
| | 1:15:39 | 75.65 | 1.89125 | 538.61 | 0.28998 | 1857.404 | 207208 | 0.008964 | -0.04104 | 2836.72 | 2006809 | 0.001414 | | 1.89125 | 0.015 |
| | 1:17:42 | 77.7 | 1.9425 | 340.99 | 0.25676 | 1328.05 | 207208 | 0.006409 | -0.04359 | 2028.264 | 2006809 | 0.001011 | | 1.9425 | 0.005 |
| | 1:19:45 | 79.75 | 1.99375 | 285.84 | 0.277 | 1031.913 | 207208 | 0.00498 | -0.04502 | 1575.99 | 2006809 | 0.000785 | | 1.99375 | 0.002 |
| | 1:21:48 | 81.8 | 2.045 | 215.72 | 0.26359 | 818.3922 | 207208 | 0.00395 | -0.04605 | 1249.889 | 2006809 | 0.000623 | | 2.045 | 0 |
| | 1:23:51 | 83.85 | 2.09625 | 188.79 | 0.27232 | 693.2653 | 207208 | 0.003346 | -0.04665 | 1058.789 | 2006809 | 0.000528 | | 2.09625 | 0 |
| | 1:25:54 | 85.9 | 2.1475 | 175.47 | 0.29226 | 600.3901 | 207208 | 0.002898 | -0.0471 | 916.9457 | 2006809 | 0.000457 | | 2.1475 | 0 |
| | 1:27:57 | 87.95 | 2.19875 | 131.69 | 0.25303 | 520.4521 | 207208 | 0.002512 | -0.04749 | 794.8605 | 2006809 | 0.000396 | | 2.19875 | 0 |
| | 1:30:00 | 90 | 2.25 | 127.32 | 0.28471 | 447.1919 | 207208 | 0.002158 | -0.04784 | 682.9738 | 2006809 | 0.00034 | | 2.25 | 0 |
| | 1:32:03 | 92.05 | 2.30125 | 121.43 | 0.29551 | 410.9167 | 207208 | 0.001983 | -0.04802 | 627.5726 | 2006809 | 0.000313 | | 2.30125 | 0 |
| | 1:34:06 | 94.1 | 2.3525 | 105.63 | 0.29847 | 353.9049 | 207208 | 0.001708 | -0.04829 | 540.5013 | 2006809 | 0.000269 | | 2.3525 | 0 |
| | 1:36:09 | 96.15 | 2.40375 | 90.74 | 0.28567 | 317.6392 | 207208 | 0.001533 | -0.04847 | 485.1145 | 2006809 | 0.000242 | | 2.40375 | 0 |
| | 1:38:12 | 98.2 | 2.455 | 74.31 | 0.25573 | 290.5799 | 207208 | 0.001402 | -0.0486 | 443.7882 | 2006809 | 0.000221 | | 2.455 | 0 |
| | | | | | | | | | | 2035991 | | 1.014541 | | | |

| 10/90% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:15:45 | 15.75 | 0.39375 | 10.43 | 0.26675 | 39.1003 | 208143 | 0.00019 | -0.09981 | 59.7159 | 2028782 | 2.9E-05 | | 0.39375 | 0 |
| slug | 0:17:48 | 17.8 | 0.445 | 17.16 | 0.28094 | 61.0807 | 208143 | 0.00029 | -0.09971 | 93.28543 | 2028782 | 4.6E-05 | | 0.445 | 0 |
| | 0:19:51 | 19.85 | 0.49625 | 73.93 | 0.29997 | 246.458 | 208143 | 0.00118 | -0.09882 | 376.4029 | 2028782 | 0.00019 | | 0.49625 | 0 |
| flow | 0:21:54 | 21.9 | 0.5475 | 236.31 | 0.26952 | 876.781 | 208143 | 0.00421 | -0.09579 | 1339.064 | 2028782 | 0.00066 | | 0.5475 | 0 |
| 0.745 | 0:23:57 | 23.95 | 0.59875 | 638.07 | 0.30653 | 2081.59 | 208143 | 0.01 | -0.09 | 3179.109 | 2028782 | 0.00157 | | 0.59875 | 0 |
| (mL/min) | 0:26:00 | 26 | 0.65 | 1023.02 | 0.27701 | 3693.08 | 208143 | 0.01774 | -0.08226 | 5640.256 | 2028782 | 0.00278 | | 0.65 | 0 |
| | 0:28:03 | 28.05 | 0.70125 | 1512.37 | 0.26163 | 5780.57 | 208143 | 0.02777 | -0.07223 | 8828.372 | 2028782 | 0.00435 | | 0.70125 | 0 |
| | 0:30:06 | 30.1 | 0.7525 | 2233.84 | 0.26682 | 8372.09 | 208143 | 0.04022 | -0.05978 | 12786.27 | 2028782 | 0.0063 | | 0.7525 | 0 |
| | 0:32:09 | 32.15 | 0.80375 | 2885.55 | 0.26693 | 10810.1 | 208143 | 0.05194 | -0.04806 | 16509.78 | 2028782 | 0.00814 | | 0.80375 | 0 |
| | 0:34:12 | 34.2 | 0.855 | 4036.54 | 0.29827 | 13533.2 | 208143 | 0.06502 | -0.03498 | 20668.54 | 2028782 | 0.01019 | | 0.855 | 0 |
| | 0:36:15 | 36.25 | 0.90625 | 4283.46 | 0.26988 | 15871.7 | 208143 | 0.07625 | -0.02375 | 24240.09 | 2028782 | 0.01195 | | 0.90625 | 0 |
| | 0:38:18 | 38.3 | 0.9575 | 5083.34 | 0.27238 | 18662.7 | 208143 | 0.08966 | -0.01034 | 28502.57 | 2028782 | 0.01405 | | 0.9575 | 0.001 |
| | 0:40:21 | 40.35 | 1.00875 | 5662.96 | 0.28933 | 19572.7 | 208143 | 0.09403 | -0.00597 | 29892.36 | 2028782 | 0.01473 | | 1.00875 | 0.004 |
| | 0:42:24 | 42.4 | 1.06 | 5495.62 | 0.25925 | 21198.1 | 208143 | 0.10184 | 0.00184 | 32374.87 | 2028782 | 0.01596 | | 1.06 | 0.018 |
| | 0:44:27 | 44.45 | 1.11125 | 6167.46 | 0.28476 | 21658.4 | 208143 | 0.10406 | 0.00406 | 33077.87 | 2028782 | 0.0163 | | 1.11125 | 0.063 |
| | 0:46:30 | 46.5 | 1.1625 | 7334.39 | 0.26052 | 28152.9 | 208143 | 0.13526 | 0.03526 | 42996.5 | 2028782 | 0.02119 | | 1.1625 | 0.16 |
| | 0:48:33 | 48.55 | 1.21375 | 15052.7 | 0.26506 | 56789.9 | 208143 | 0.27284 | 0.17284 | 86732.43 | 2028782 | 0.04275 | | 1.21375 | 0.313 |
| | 0:50:36 | 50.6 | 1.265 | 28886.4 | 0.27691 | 104317 | 208143 | 0.50118 | 0.40118 | 159317.8 | 2028782 | 0.07853 | | 1.265 | 0.498 |
| | 0:52:39 | 52.65 | 1.31625 | 36744.1 | 0.24763 | 148383 | 208143 | 0.71289 | 0.61289 | 226618.2 | 2028782 | 0.1117 | | 1.31625 | 0.676 |
| | 0:54:42 | 54.7 | 1.3675 | 45284.1 | 0.26458 | 171155 | 208143 | 0.82229 | 0.72229 | 261396 | 2028782 | 0.12884 | | 1.3675 | 0.81 |
| | 0:56:45 | 56.75 | 1.41875 | 51379.9 | 0.27252 | 188536 | 208143 | 0.9058 | 0.8058 | 287942.1 | 2028782 | 0.14193 | | 1.41875 | 0.871 |
| | 0:58:48 | 58.8 | 1.47 | 46316 | 0.26381 | 175566 | 208143 | 0.84349 | 0.74349 | 268132.6 | 2028782 | 0.13216 | | 1.47 | 0.848 |
| | 1:00:51 | 60.85 | 1.52125 | 39669 | 0.26615 | 149048 | 208143 | 0.71608 | 0.61608 | 227632.8 | 2028782 | 0.1122 | | 1.52125 | 0.741 |
| | 1:02:54 | 62.9 | 1.5725 | 36759.8 | 0.29091 | 126361 | 208143 | 0.60709 | 0.50709 | 192985.4 | 2028782 | 0.09512 | | 1.5725 | 0.571 |
| | 1:04:57 | 64.95 | 1.62375 | 23588.9 | 0.27723 | 85087.9 | 208143 | 0.4088 | 0.3088 | 129950.6 | 2028782 | 0.06405 | | 1.62375 | 0.388 |
| | 1:07:00 | 67 | 1.675 | 10284.6 | 0.26285 | 39127.3 | 208143 | 0.18798 | 0.08798 | 59757.22 | 2028782 | 0.02945 | | 1.675 | 0.231 |
| | 1:09:03 | 69.05 | 1.72625 | 3659.91 | 0.28617 | 12789.3 | 208143 | 0.06144 | -0.03856 | 19532.44 | 2028782 | 0.00963 | | 1.72625 | 0.12 |
| | 1:11:06 | 71.1 | 1.7775 | 1205.7 | 0.26525 | 4545.52 | 208143 | 0.02184 | -0.07816 | 6942.15 | 2028782 | 0.00342 | | 1.7775 | 0.055 |
| | 1:13:09 | 73.15 | 1.82875 | 659.86 | 0.27571 | 2393.31 | 208143 | 0.0115 | -0.0885 | 3655.185 | 2028782 | 0.0018 | | 1.82875 | 0.022 |
| | 1:15:12 | 75.2 | 1.88 | 473.33 | 0.2879 | 1644.08 | 208143 | 0.0079 | -0.0921 | 2510.918 | 2028782 | 0.00124 | | 1.88 | 0.008 |
| | 1:17:15 | 77.25 | 1.93125 | 349.07 | 0.26919 | 1296.74 | 208143 | 0.00623 | -0.09377 | 1980.449 | 2028782 | 0.00098 | | 1.93125 | 0.003 |
| | 1:19:18 | 79.3 | 1.9825 | 344.2 | 0.29353 | 1172.62 | 208143 | 0.00563 | -0.09437 | 1790.888 | 2028782 | 0.00088 | | 1.9825 | 0.001 |
| | 1:21:21 | 81.35 | 2.03375 | 290.18 | 0.27532 | 1053.97 | 208143 | 0.00506 | -0.09494 | 1609.681 | 2028782 | 0.00079 | | 2.03375 | 0 |
| | 1:23:24 | 83.4 | 2.085 | 235.91 | 0.263 | 896.996 | 208143 | 0.00431 | -0.09569 | 1369.937 | 2028782 | 0.00068 | | 2.085 | 0 |
| | 1:25:27 | 85.45 | 2.13625 | 208.45 | 0.27736 | 751.55 | 208143 | 0.00361 | -0.09639 | 1147.805 | 2028782 | 0.00057 | | 2.13625 | 0 |
| | 1:27:30 | 87.5 | 2.1875 | 163.46 | 0.26006 | 628.547 | 208143 | 0.00302 | -0.09698 | 959.9488 | 2028782 | 0.00047 | | 2.1875 | 0 |
| | 1:29:33 | 89.55 | 2.23875 | 146.76 | 0.27245 | 538.668 | 208143 | 0.00259 | -0.09741 | 822.6802 | 2028782 | 0.00041 | | 2.23875 | 0 |
| | 1:31:36 | 91.6 | 2.29 | 129 | 0.27374 | 471.25 | 208143 | 0.00226 | -0.09774 | 719.7167 | 2028782 | 0.00035 | | 2.29 | 0 |
| | 1:33:39 | 93.65 | 2.34125 | 105.6 | 0.27264 | 387.324 | 208143 | 0.00186 | -0.09814 | 591.5405 | 2028782 | 0.00029 | | 2.34125 | 0 |
| | 1:35:42 | 95.7 | 2.3925 | 93.76 | 0.26758 | 350.4 | 208143 | 0.00168 | -0.09832 | 535.1482 | 2028782 | 0.00026 | | 2.3925 | 0 |
| | | | | | | | | | | 2205199 | | 1.08696 | | | |

| 20/80% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:17:35 | 17.58333 | 0.439583 | 4454.08 | 0.27035 | 16475.24 | 194936 | 0.084516 | 0.054516 | 25161.8 | 1875858 | 0.013413 | | 0.439583 | 0 |
| slug | 0:19:38 | 19.63333 | 0.490833 | 4836.74 | 0.26027 | 18583.55 | 194936 | 0.095332 | 0.065332 | 28381.72 | 1875858 | 0.01513 | | 0.490833 | 0 |
| | 0:21:41 | 21.68333 | 0.542083 | 4745.58 | 0.27941 | 16984.29 | 194936 | 0.087128 | 0.057128 | 25939.25 | 1875858 | 0.013828 | | 0.542083 | 0 |
| flow | 0:23:44 | 23.73333 | 0.593333 | 4114.73 | 0.30475 | 13501.99 | 194936 | 0.069264 | 0.039264 | 20620.91 | 1875858 | 0.010993 | | 0.593333 | 0 |
| 0.745 | 0:25:47 | 25.78333 | 0.644583 | 2983.67 | 0.25697 | 11610.97 | 194936 | 0.059563 | 0.029563 | 17732.85 | 1875858 | 0.009453 | | 0.644583 | 0 |
| (mL/min) | 0:27:50 | 27.83333 | 0.695833 | 2738.25 | 0.2808 | 9751.603 | 194936 | 0.050025 | 0.020025 | 14893.14 | 1875858 | 0.007939 | | 0.695833 | 0 |
| | 0:29:53 | 29.88333 | 0.747083 | 2443.11 | 0.29083 | 8400.475 | 194936 | 0.043093 | 0.013093 | 12829.62 | 1875858 | 0.006839 | | 0.747083 | 0 |
| | 0:31:56 | 31.93333 | 0.798333 | 2324.43 | 0.29098 | 7988.281 | 194936 | 0.040979 | 0.010979 | 12200.1 | 1875858 | 0.006504 | | 0:798333 | 0 |
| | 0:33:59 | 33.98333 | 0.849583 | 2109.95 | 0.28872 | 7307.945 | 194936 | 0.037489 | 0.007489 | 11161.06 | 1875858 | 0.00595 | | 0.849583 | 0 |
| | 0:36:02 | 36.03333 | 0.900833 | 1965.31 | 0.26784 | 7337.627 | 194936 | 0.037641 | 0.007641 | 11206.39 | 1875858 | 0.005974 | | 0.900833 | 0 |
| | 0:38:05 | 38.08333 | 0.952083 | 1671.6 | 0.24671 | 6775.566 | 194936 | 0.034758 | 0.004758 | 10347.98 | 1875858 | 0.005516 | | 0.952083 | 0 |
| | 0:40:08 | 40.13333 | 1.003333 | 1710.34 | 0.26998 | 6335.062 | 194936 | 0.032498 | 0.002498 | 9675.223 | 1875858 | 0.005158 | | 1.003333 | 0 |
| | 0:42:11 | 42.18333 | 1.054583 | 1768.33 | 0.2862 | 6178.651 | 194936 | 0.031696 | 0.001696 | 9436.345 | 1875858 | 0.00503 | | 1.054583 | 0 |
| | 0:44:14 | 44.23333 | 1.105833 | 1887.65 | 0.30551 | 6178.685 | 194936 | 0.031696 | 0.001696 | 9436.396 | 1875858 | 0.00503 | | 1.105833 | 0.001 |
| | 0:46:17 | 46.28333 | 1.157083 | 1915.83 | 0.28615 | 6695.195 | 194936 | 0.034346 | 0.004346 | 10225.24 | 1875858 | 0.005451 | | 1.157083 | 0.005 |
| | 0:48:20 | 48.33333 | 1.208333 | 2851.36 | 0.30956 | 9211.009 | 194936 | 0.047251 | 0.017251 | 14067.51 | 1875858 | 0.007499 | | 1.208333 | 0.023 |
| | 0:50:23 | 50.38333 | 1.259583 | 4477.44 | 0.25374 | 17645.78 | 194936 | 0.090521 | 0.060521 | 26949.52 | 1875858 | 0.014367 | | 1.259583 | 0.074 |
| | 0:52:26 | 52.43333 | 1.310833 | 10936.48 | 0.27914 | 39179.19 | 194936 | 0.200985 | 0.170985 | 59836.42 | 1875858 | 0.031898 | | 1.310833 | 0.174 |
| | 0:54:29 | 54.48333 | 1.362083 | 16805.85 | 0.23939 | 70202.81 | 194936 | 0.360133 | 0.330133 | 107217.2 | 1875858 | 0.057156 | | 1.362083 | 0.326 |
| | 0:56:32 | 56.53333 | 1.413333 | 30119.62 | 0.27699 | 108739 | 194936 | 0.557819 | 0.527819 | 166071.7 | 1875858 | 0.088531 | | 1.413333 | 0.508 |
| | 0:58:35 | 58.58333 | 1.464583 | 38010.49 | 0.26573 | 143041.8 | 194936 | 0.733788 | 0.703788 | 218460.5 | 1875858 | 0.116459 | | 1.464583 | 0.683 |
| | 1:00:38 | 60.63333 | 1.515833 | 46455.3 | 0.29129 | 159481.3 | 194936 | 0.818121 | 0.788121 | 243567.8 | 1875858 | 0.129843 | | 1.515833 | 0.806 |
| | 1:02:41 | 62.68333 | 1.567083 | 39179.64 | 0.23582 | 166142.1 | 194936 | 0.852291 | 0.822291 | 253740.6 | 1875858 | 0.135266 | | 1.567083 | 0.857 |
| | 1:04:44 | 64.73333 | 1.618333 | 41194.68 | 0.26956 | 152821.9 | 194936 | 0.78396 | 0.75396 | 233397.3 | 1875858 | 0.124422 | | 1.618333 | 0.823 |
| | 1:06:47 | 66.78333 | 1.669583 | 37050.2 | 0.25161 | 147252.5 | 194936 | 0.755389 | 0.725389 | 224891.4 | 1875858 | 0.119887 | | 1.669583 | 0.705 |
| | 1:08:50 | 68.83333 | 1.720833 | 32546.08 | 0.26773 | 121563.1 | 194936 | 0.623605 | 0.593605 | 185657.2 | 1875858 | 0.098972 | | 1.720833 | 0.537 |
| | 1:10:53 | 70.88333 | 1.772083 | 25788.14 | 0.29943 | 86124.1 | 194936 | 0.441807 | 0.411807 | 131533 | 1875858 | 0.070119 | | 1.772083 | 0.36 |
| | 1:12:56 | 72.93333 | 1.823333 | 10689.85 | 0.26672 | 40078.92 | 194936 | 0.2056 | 0.1756 | 61210.53 | 1875858 | 0.032631 | | 1.823333 | 0.212 |
| | 1:14:59 | 74.98333 | 1.874583 | 3907.36 | 0.27791 | 14059.8 | 194936 | 0.072125 | 0.042125 | 21472.83 | 1875858 | 0.011447 | | 1.874583 | 0.109 |
| | 1:17:02 | 77.03333 | 1.925833 | 1444.33 | 0.28099 | 5140.147 | 194936 | 0.026368 | -0.00363 | 7850.29 | 1875858 | 0.004185 | | 1.925833 | 0.05 |
| | 1:19:05 | 79.08333 | 1.977083 | 721.28 | 0.24233 | 2976.437 | 194936 | 0.015269 | -0.01473 | 4545.764 | 1875858 | 0.002423 | | 1.977083 | 0.02 |
| | 1:21:08 | 81.13333 | 2.028333 | 529.54 | 0.24083 | 2198.812 | 194936 | 0.01128 | -0.01872 | 3358.136 | 1875858 | 0.00179 | | 2.028333 | 0.007 |
| | 1:23:11 | 83.18333 | 2.079583 | 477.04 | 0.28379 | 1680.961 | 194936 | 0.008623 | -0.02138 | 2567.248 | 1875858 | 0.001369 | | 2.079583 | 0.002 |
| | 1:25:14 | 85.23333 | 2.130833 | 372.4 | 0.27904 | 1334.576 | 194936 | 0.006846 | -0.02315 | 2038.231 | 1875858 | 0.001087 | | 2.130833 | 0.001 |
| | 1:27:17 | 87.28333 | 2.182083 | 278.78 | 0.25094 | 1110.943 | 194936 | 0.005699 | -0.0243 | 1696.687 | 1875858 | 0.000904 | | 2.182083 | 0 |
| | 1:29:20 | 89.33333 | 2.233333 | 261.16 | 0.27466 | 950.8483 | 194936 | 0.004878 | -0.02512 | 1452.183 | 1875858 | 0.000774 | | 2.233333 | 0 |
| | 1:31:23 | 91.38333 | 2.284583 | 232.67 | 0.28134 | 827.0065 | 194936 | 0.004242 | -0.02576 | 1263.046 | 1875858 | 0.000673 | | 2.284583 | 0 |
| | 1:33:26 | 93.43333 | 2.335833 | 183.17 | 0.23985 | 763.6856 | 194936 | 0.003918 | -0.02608 | 1166.339 | 1875858 | 0.000622 | | 2.335833 | 0 |
| | 1:35:29 | 95.48333 | 2.387083 | 179.1 | 0.2583 | 693.3798 | 194936 | 0.003557 | -0.02644 | 1058.964 | 1875858 | 0.000565 | | 2.387083 | 0 |
| | 1:37:32 | 97.53333 | 2.438333 | 161.33 | 0.27979 | 576.611 | 194936 | 0.002958 | -0.02704 | 880.6292 | 1875858 | 0.000469 | | 2.438333 | 0 |
| | | | | | | | | | | 2205199 | | 1.175568 | | | |

| 50/50% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | Adj C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| meth | 0:16:15 | 16.25 | 0.40625 | 2364.69 | 0.28663 | 8249.974 | 201759 | 0.04089 | 0.00089 | 12599.77 | 1991614 | 0.006326 | | 0.40625 | 0 |
| slug | 0:18:18 | 18.3 | 0.4575 | 2529.82 | 0.26911 | 9400.691 | 201759 | 0.046594 | 0.006594 | 14357.21 | 1991614 | 0.007209 | | 0.4575 | 0 |
| | 0:20:21 | 20.35 | 0.50875 | 2969.27 | 0.26909 | 11034.49 | 201759 | 0.054691 | 0.014691 | 16852.42 | 1991614 | 0.008462 | | 0.50875 | 0 |
| flow | 0:22:24 | 22.4 | 0.56 | 2950.22 | 0.25981 | 11355.3 | 201759 | 0.056281 | 0.016281 | 17342.38 | 1991614 | 0.008708 | | 0.56 | 0 |
| 0.745 | 0:24:27 | 24.45 | 0.61125 | 2739.26 | 0.27512 | 9956.601 | 201759 | 0.049349 | 0.009349 | 15206.22 | 1991614 | 0.007635 | | 0.61125 | 0 |
| (mL/min) | 0:26:30 | 26.5 | 0.6625 | 2409 | 0.28455 | 8465.999 | 201759 | 0.041961 | 0.001961 | 12929.7 | 1991614 | 0.006492 | | 0.6625 | 0 |
| | 0:28:33 | 28.55 | 0.71375 | 2042.21 | 0.28475 | 7171.94 | 201759 | 0.035547 | -0.00445 | 10953.35 | 1991614 | 0.0055 | | 0.71375 | 0 |
| | 0:30:36 | 30.6 | 0.765 | 1954.81 | 0.27844 | 7020.579 | 201759 | 0.034797 | -0.0052 | 10722.18 | 1991614 | 0.005384 | | 0.765 | 0 |
| | 0:32:39 | 32.65 | 0.81625 | 1842.34 | 0.26984 | 6827.527 | 201759 | 0.03384 | -0.00616 | 10427.34 | 1991614 | 0.005236 | | 0.81625 | 0 |
| | 0:34:42 | 34.7 | 0.8675 | 2009.9 | 0.315 | 6380.635 | 201759 | 0.031625 | -0.00837 | 9744.825 | 1991614 | 0.004893 | | 0.8675 | 0 |
| | 0:36:45 | 36.75 | 0.91875 | 1677.56 | 0.26949 | 6224.943 | 201759 | 0.030853 | -0.00915 | 9507.045 | 1991614 | 0.004774 | | 0.91875 | 0 |
| | 0:38:48 | 38.8 | 0.97 | 1515.55 | 0.2818 | 5378.105 | 201759 | 0.026656 | -0.01334 | 8213.711 | 1991614 | 0.004124 | | 0.97 | 0 |
| | 0:40:51 | 40.85 | 1.02125 | 1375.44 | 0.26074 | 5275.14 | 201759 | 0.026146 | -0.01385 | 8056.458 | 1991614 | 0.004045 | | 1.02125 | 0.001 |
| | 0:42:54 | 42.9 | 1.0725 | 1608.26 | 0.29565 | 5439.743 | 201759 | 0.026962 | -0.01304 | 8307.847 | 1991614 | 0.004171 | | 1.0725 | 0.005 |
| | 0:44:57 | 44.95 | 1.12375 | 1973.91 | 0.29873 | 6607.672 | 201759 | 0.03275 | -0.00725 | 10091.57 | 1991614 | 0.005067 | | 1.12375 | 0.018 |
| | 0:47:00 | 47 | 1.175 | 3033.58 | 0.26071 | 11635.84 | 201759 | 0.057672 | 0.017672 | 17770.84 | 1991614 | 0.008923 | | 1.175 | 0.052 |
| | 0:49:03 | 49.05 | 1.22625 | 7000.35 | 0.29172 | 23996.81 | 201759 | 0.118938 | 0.078938 | 36649.13 | 1991614 | 0.018402 | | 1.22625 | 0.119 |
| | 0:51:06 | 51.1 | 1.2775 | 15689.03 | 0.2912 | 53877.16 | 201759 | 0.267037 | 0.227037 | 82283.9 | 1991614 | 0.041315 | | 1.2775 | 0.23 |
| | 0:53:09 | 53.15 | 1.32875 | 24200.7 | 0.27575 | 87763.19 | 201759 | 0.43499 | 0.39499 | 134036.3 | 1991614 | 0.0673 | | 1.32875 | 0.371 |
| | 0:55:12 | 55.2 | 1.38 | 35330.47 | 0.27012 | 130795.5 | 201759 | 0.648276 | 0.608276 | 199757.4 | 1991614 | 0.100299 | | 1.38 | 0.525 |
| | 0:57:15 | 57.25 | 1.43125 | 37955.98 | 0.24936 | 152213.6 | 201759 | 0.754433 | 0.714433 | 232468.2 | 1991614 | 0.116724 | | 1.43125 | 0.664 |
| | 0:59:18 | 59.3 | 1.4825 | 42188.05 | 0.27572 | 153010.5 | 201759 | 0.758382 | 0.718382 | 233685.3 | 1991614 | 0.117335 | | 1.4825 | 0.763 |
| | 1:01:21 | 61.35 | 1.53375 | 42861.35 | 0.27758 | 154410.8 | 201759 | 0.765323 | 0.725323 | 235823.9 | 1991614 | 0.118408 | | 1.53375 | 0.798 |
| | 1:03:24 | 63.4 | 1.585 | 41323.98 | 0.27144 | 152239.8 | 201759 | 0.754563 | 0.714563 | 232508.3 | 1991614 | 0.116744 | | 1.585 | 0.763 |
| | 1:05:27 | 65.45 | 1.63625 | 41121.33 | 0.2832 | 145202.4 | 201759 | 0.719683 | 0.679683 | 221760.4 | 1991614 | 0.111347 | | 1.63625 | 0.667 |
| | 1:07:30 | 67.5 | 1.6875 | 32974.48 | 0.25616 | 128726.1 | 201759 | 0.638019 | 0.598019 | 196596.9 | 1991614 | 0.098712 | | 1.6875 | 0.529 |
| | 1:09:33 | 69.55 | 1.73875 | 27193.33 | 0.26041 | 104425.1 | 201759 | 0.517573 | 0.477573 | 159483.2 | 1991614 | 0.080077 | | 1.73875 | 0.383 |
| | 1:11:36 | 71.6 | 1.79 | 14820.36 | 0.24022 | 61694.95 | 201759 | 0.305785 | 0.265785 | 94223.61 | 1991614 | 0.04731 | | 1.79 | 0.253 |
| | 1:13:39 | 73.65 | 1.84125 | 6962.68 | 0.25181 | 27650.53 | 201759 | 0.137047 | 0.097047 | 42229.27 | 1991614 | 0.021204 | | 1.84125 | 0.153 |
| | 1:15:42 | 75.7 | 1.8925 | 3175.93 | 0.26964 | 11778.41 | 201759 | 0.058379 | 0.018379 | 17988.57 | 1991614 | 0.009032 | | 1.8925 | 0.084 |
| | 1:17:45 | 77.75 | 1.94375 | 1546.22 | 0.24612 | 6282.383 | 201759 | 0.031138 | -0.00886 | 9594.769 | 1991614 | 0.004818 | | 1.94375 | 0.043 |
| | 1:19:48 | 79.8 | 1.995 | 1048.95 | 0.26105 | 4018.196 | 201759 | 0.019916 | -0.02008 | 6136.789 | 1991614 | 0.003081 | | 1.995 | 0.02 |
| | 1:21:51 | 81.85 | 2.04625 | 733.27 | 0.25911 | 2829.956 | 201759 | 0.014026 | -0.02597 | 4322.051 | 1991614 | 0.00217 | | 2.04625 | 0.009 |
| | 1:23:54 | 83.9 | 2.0975 | 558.25 | 0.26328 | 2120.366 | 201759 | 0.010509 | -0.02949 | 3238.329 | 1991614 | 0.001626 | | 2.0975 | 0.004 |
| | 1:25:57 | 85.95 | 2.14875 | 430.55 | 0.2525 | 1705.149 | 201759 | 0.008451 | -0.03155 | 2604.188 | 1991614 | 0.001308 | | 2.14875 | 0.001 |
| | 1:28:00 | 88 | 2.2 | 394.57 | 0.26412 | 1493.904 | 201759 | 0.007404 | -0.0326 | 2281.565 | 1991614 | 0.001146 | | 2.2 | 0.001 |
| | 1:30:03 | 90.05 | 2.25125 | 349.32 | 0.26394 | 1323.483 | 201759 | 0.00656 | -0.03344 | 2021.289 | 1991614 | 0.001015 | | 2.25125 | 0 |
| | 1:32:06 | 92.1 | 2.3025 | 295.81 | 0.25511 | 1159.539 | 201759 | 0.005747 | -0.03425 | 1770.906 | 1991614 | 0.000889 | | 2.3025 | 0 |
| | 1:34:09 | 94.15 | 2.35375 | 270.49 | 0.26514 | 1020.178 | 201759 | 0.005056 | -0.03494 | 1558.067 | 1991614 | 0.000782 | | 2.35375 | 0 |
| | 1:36:12 | 96.2 | 2.405 | 237.34 | 0.24317 | 976.025 | 201759 | 0.004838 | -0.03516 | 1490.634 | 1991614 | 0.000748 | | 2.405 | 0 |
| | | | | | | | | | | 2347596 | | 1.178741 | | | |

| 0/100% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:22:05 | 22.0833 | 0.55208 | 1.58 | 0.29922 | 5.2804 | 312928 | 1.7E-05 | 8.06448 | 3100647 | 2.6E-06 | | 0.55208 | 0 |
| tracer | 0:24:08 | 24.1333 | 0.60333 | 1.62 | 0.31203 | 5.19181 | 312928 | 1.7E-05 | 7.92919 | 3100647 | 2.6E-06 | | 0.60333 | 0 |
| | 0:26:11 | 26.1833 | 0.65458 | 2.55 | 0.34117 | 7.47428 | 312928 | 2.4E-05 | 11.4151 | 3100647 | 3.7E-06 | | 0.65458 | 0 |
| flow | 0:28:14 | 28.2333 | 0.70583 | 1.22 | 0.31864 | 3.82877 | 312928 | 1.2E-05 | 5.84749 | 3100647 | 1.9E-06 | | 0.70583 | 0 |
| 0.745 | 0:30:17 | 30.2833 | 0.75708 | 1.24 | 0.29294 | 4.23295 | 312928 | 1.4E-05 | 6.46477 | 3100647 | 2.1E-06 | | 0.75708 | 0 |
| (mL/min) | 0:32:20 | 32.3333 | 0.80833 | 3.42 | 0.21302 | 16.0548 | 312928 | 5.1E-05 | 24.5197 | 3100647 | 7.9E-06 | | 0.80833 | 0 |
| | 0:34:23 | 34.3833 | 0.85958 | 2.19 | 0.25764 | 8.50023 | 312928 | 2.7E-05 | 12.982 | 3100647 | 4.2E-06 | | 0.85958 | 0.001 |
| | 0:36:26 | 36.4333 | 0.91083 | 7.83 | 0.25761 | 30.3948 | 312928 | 9.7E-05 | 46.4204 | 3100647 | 1.5E-05 | | 0.91083 | 0.007 |
| | 0:38:29 | 38.4833 | 0.96208 | 47.2 | 0.29477 | 160.125 | 312928 | 0.00051 | 244.551 | 3100647 | 7.9E-05 | | 0.96208 | 0.025 |
| | 0:40:32 | 40.5333 | 1.01333 | 166.42 | 0.25354 | 656.386 | 312928 | 0.0021 | 1002.46 | 3100647 | 0.00032 | | 1.01333 | 0.067 |
| | 0:42:35 | 42.5833 | 1.06458 | 514.08 | 0.19449 | 2643.22 | 312928 | 0.00845 | 4036.86 | 3100647 | 0.0013 | | 1.06458 | 0.147 |
| | 0:44:38 | 44.6333 | 1.11583 | 5644.13 | 0.30219 | 18677.4 | 312928 | 0.05969 | 28525.1 | 3100647 | 0.0092 | | 1.11583 | 0.264 |
| | 0:46:41 | 46.6833 | 1.16708 | 25757.7 | 0.28488 | 90415.8 | 312928 | 0.28893 | 138088 | 3100647 | 0.04454 | | 1.16708 | 0.408 |
| | 0:48:44 | 48.7333 | 1.21833 | 47379.4 | 0.25282 | 187404 | 312928 | 0.59887 | 286212 | 3100647 | 0.09231 | | 1.21833 | 0.557 |
| | 0:50:47 | 50.7833 | 1.26958 | 60604 | 0.23892 | 253658 | 312928 | 0.8106 | 387400 | 3100647 | 0.12494 | | 1.26958 | 0.686 |
| | 0:52:50 | 52.8333 | 1.32083 | 78574.5 | 0.27504 | 285684 | 312928 | 0.91294 | 436311 | 3100647 | 0.14072 | | 1.32083 | 0.768 |
| | 0:54:53 | 54.8833 | 1.37208 | 79118.9 | 0.26643 | 296959 | 312928 | 0.94897 | 453531 | 3100647 | 0.14627 | | 1.37208 | 0.788 |
| | 0:56:56 | 56.9333 | 1.42333 | 84891.9 | 0.29374 | 289004 | 312928 | 0.92355 | 441381 | 3100647 | 0.14235 | | 1.42333 | 0.741 |
| | 0:58:59 | 58.9833 | 1.47458 | 60228.6 | 0.25985 | 231782 | 312928 | 0.74069 | 353989 | 3100647 | 0.11417 | | 1.47458 | 0.637 |
| | 1:01:02 | 61.0333 | 1.52583 | 40149.2 | 0.27298 | 147077 | 312928 | 0.47 | 224624 | 3100647 | 0.07244 | | 1.52583 | 0.502 |
| | 1:03:05 | 63.0833 | 1.57708 | 22348.6 | 0.29799 | 74997.9 | 312928 | 0.23966 | 114541 | 3100647 | 0.03694 | | 1.57708 | 0.363 |
| | 1:05:08 | 65.1333 | 1.62833 | 9608.05 | 0.2612 | 36784.3 | 312928 | 0.11755 | 56178.8 | 3100647 | 0.01812 | | 1.62833 | 0.242 |
| | 1:07:11 | 67.1833 | 1.67958 | 4556.66 | 0.27898 | 16333.3 | 312928 | 0.0522 | 24945 | 3100647 | 0.00805 | | 1.67958 | 0.147 |
| | 1:09:14 | 69.2333 | 1.73083 | 2170.69 | 0.2657 | 8169.7 | 312928 | 0.02611 | 12477.2 | 3100647 | 0.00402 | | 1.73083 | 0.084 |
| | 1:11:17 | 71.2833 | 1.78208 | 1464.84 | 0.29216 | 5013.83 | 312928 | 0.01602 | 7657.37 | 3100647 | 0.00247 | | 1.78208 | 0.044 |
| | 1:13:20 | 73.3333 | 1.83333 | 1365.88 | 0.35375 | 3861.14 | 312928 | 0.01234 | 5896.93 | 3100647 | 0.0019 | | 1.83333 | 0.022 |
| | 1:15:23 | 75.3833 | 1.88458 | 950.79 | 0.295 | 3223.02 | 312928 | 0.0103 | 4922.35 | 3100647 | 0.00159 | | 1.88458 | 0.01 |
| | 1:17:26 | 77.4333 | 1.93583 | 768.2 | 0.27559 | 2787.47 | 312928 | 0.00891 | 4257.17 | 3100647 | 0.00137 | | 1.93583 | 0.005 |
| | 1:19:29 | 79.4833 | 1.98708 | 831.4 | 0.34071 | 2440.2 | 312928 | 0.0078 | 3726.79 | 3100647 | 0.0012 | | 1.98708 | 0.002 |
| | 1:21:32 | 81.5333 | 2.03833 | 593.07 | 0.28347 | 2092.18 | 312928 | 0.00669 | 3195.28 | 3100647 | 0.00103 | | 2.03833 | 0.001 |
| | 1:23:35 | 83.5833 | 2.08958 | 477.54 | 0.26393 | 1809.34 | 312928 | 0.00578 | 2763.32 | 3100647 | 0.00089 | | 2.08958 | 0 |
| | 1:25:38 | 85.6333 | 2.14083 | 468.82 | 0.31449 | 1490.73 | 312928 | 0.00476 | 2276.72 | 3100647 | 0.00073 | | 2.14083 | 0 |
| | 1:27:41 | 87.6833 | 2.19208 | 326.98 | 0.28926 | 1130.4 | 312928 | 0.00361 | 1726.41 | 3100647 | 0.00056 | | 2.19208 | 0 |
| | 1:29:44 | 89.7333 | 2.24333 | 265.43 | 0.30299 | 876.036 | 312928 | 0.0028 | 1337.93 | 3100647 | 0.00043 | | 2.24333 | 0 |
| | 1:31:47 | 91.7833 | 2.29458 | 223.11 | 0.32482 | 686.873 | 312928 | 0.00219 | 1049.03 | 3100647 | 0.00034 | | 2.29458 | 0 |
| | 1:33:50 | 93.8333 | 2.34583 | 156.13 | 0.29126 | 536.05 | 312928 | 0.00171 | 818.683 | 3100647 | 0.00026 | | 2.34583 | 0 |
| | 1:35:53 | 95.8833 | 2.39708 | 128.38 | 0.30931 | 415.053 | 312928 | 0.00133 | 633.889 | 3100647 | 0.0002 | | 2.39708 | 0 |
| | 1:37:56 | 97.9333 | 2.44833 | 92.72 | 0.26523 | 349.583 | 312928 | 0.00112 | 533.901 | 3100647 | 0.00017 | | 2.44833 | 0 |
| | 1:39:59 | 99.9833 | 2.49958 | 84.69 | 0.27667 | 306.105 | 312928 | 0.00098 | 467.498 | 3100647 | 0.00015 | | 2.49958 | 0 |
| | 1:42:02 | 102.033 | 2.55083 | 76.42 | 0.29163 | 262.044 | 312928 | 0.00084 | 400.207 | 3100647 | 0.00013 | | 2.55083 | 0 |
| | | | | | | | | | 3005273 | | 0.96924 | | | |

| 1/99% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:20:10 | 20.16667 | 0.504167 | 6.23 | 0.2993 | 20.81524 | 300088 | 6.94E-05 | 31.79007 | 3018135 | 1.05E-05 | | 0.504167 | 0 |
| mobil. | 0:22:13 | 22.21667 | 0.555417 | 13.5 | 0.32692 | 41.29451 | 300088 | 0.000138 | 63.06703 | 3018135 | 2.09E-05 | | 0.555417 | 0 |
| | 0:24:16 | 24.26667 | 0.606667 | 41.95 | 0.30077 | 139.4753 | 300088 | 0.000465 | 213.0137 | 3018135 | 7.06E-05 | | 0.606667 | 0 |
| flow | 0:26:19 | 26.31667 | 0.657917 | 110.61 | 0.28692 | 385.5082 | 300088 | 0.001285 | 588.7673 | 3018135 | 0.000195 | | 0.657917 | 0 |
| 0.745 | 0:28:22 | 28.36667 | 0.709167 | 274.83 | 0.32678 | 841.0245 | 300088 | 0.002803 | 1284.455 | 3018135 | 0.000426 | | 0.709167 | 0 |
| (mL/min) | 0:30:25 | 30.41667 | 0.760417 | 522.43 | 0.30691 | 1702.225 | 300088 | 0.005672 | 2599.724 | 3018135 | 0.000861 | | 0.760417 | 0 |
| | 0:32:28 | 32.46667 | 0.811667 | 861.5 | 0.29139 | 2956.519 | 300088 | 0.009852 | 4515.343 | 3018135 | 0.001496 | | 0.811667 | 0 |
| | 0:34:31 | 34.51667 | 0.862917 | 1556.16 | 0.31419 | 4952.927 | 300088 | 0.016505 | 7564.357 | 3018135 | 0.002506 | | 0.862917 | 0.001 |
| | 0:36:34 | 36.56667 | 0.914167 | 2229.99 | 0.3014 | 7398.772 | 300088 | 0.024655 | 11299.78 | 3018135 | 0.003744 | | 0.914167 | 0.005 |
| | 0:38:37 | 38.61667 | 0.965417 | 3410.41 | 0.31696 | 10759.75 | 300088 | 0.035855 | 16432.83 | 3018135 | 0.005445 | | 0.965417 | 0.019 |
| | 0:40:40 | 40.66667 | 1.016667 | 4963.57 | 0.31184 | 15917.04 | 300088 | 0.053041 | 24309.3 | 3018135 | 0.008054 | | 1.016667 | 0.055 |
| | 0:42:43 | 42.71667 | 1.067917 | 7178.51 | 0.29156 | 24621.04 | 300088 | 0.082046 | 37602.48 | 3018135 | 0.012459 | | 1.067917 | 0.121 |
| | 0:44:46 | 44.76667 | 1.119167 | 12928.73 | 0.30482 | 42414.31 | 300088 | 0.14134 | 64777.26 | 3018135 | 0.021463 | | 1.119167 | 0.223 |
| | 0:46:49 | 46.81667 | 1.170417 | 23342.52 | 0.29452 | 79256.15 | 300088 | 0.26411 | 121043.9 | 3018135 | 0.040106 | | 1.170417 | 0.355 |
| | 0:48:52 | 48.86667 | 1.221667 | 40322.63 | 0.30067 | 134109.3 | 300088 | 0.4469 | 204818.4 | 3018135 | 0.067863 | | 1.221667 | 0.502 |
| | 0:50:55 | 50.91667 | 1.272917 | 61946.39 | 0.31707 | 195371.3 | 300088 | 0.651047 | 298380.9 | 3018135 | 0.098863 | | 1.272917 | 0.634 |
| | 0:52:58 | 52.96667 | 1.324167 | 76281.41 | 0.29659 | 257194.8 | 300088 | 0.857065 | 392800.8 | 3018135 | 0.130147 | | 1.324167 | 0.732 |
| | 0:55:01 | 55.01667 | 1.375417 | 81202.03 | 0.30404 | 267076.8 | 300088 | 0.889995 | 407893 | 3018135 | 0.135147 | | 1.375417 | 0.775 |
| | 0:57:04 | 57.06667 | 1.426667 | 74733.41 | 0.28129 | 265681 | 300088 | 0.885344 | 405761.3 | 3018135 | 0.134441 | | 1.426667 | 0.755 |
| | 0:59:07 | 59.11667 | 1.477917 | 72148.01 | 0.30984 | 232855.7 | 300088 | 0.775958 | 355628.9 | 3018135 | 0.117831 | | 1.477917 | 0.676 |
| | 1:01:10 | 61.16667 | 1.529167 | 61333.12 | 0.32483 | 188816.1 | 300088 | 0.629202 | 288369.3 | 3018135 | 0.095546 | | 1.529167 | 0.558 |
| | 1:03:13 | 63.21667 | 1.580417 | 40176.09 | 0.32152 | 124956.7 | 300088 | 0.4164 | 190840.2 | 3018135 | 0.063231 | | 1.580417 | 0.425 |
| | 1:05:16 | 65.26667 | 1.631667 | 18182.75 | 0.3021 | 60187.85 | 300088 | 0.200567 | 91921.9 | 3018135 | 0.030457 | | 1.631667 | 0.296 |
| | 1:07:19 | 67.31667 | 1.682917 | 5698.56 | 0.26194 | 21755.21 | 300088 | 0.072496 | 33225.65 | 3018135 | 0.011009 | | 1.682917 | 0.193 |
| | 1:09:22 | 69.36667 | 1.734167 | 2055.15 | 0.30128 | 6821.395 | 300088 | 0.022731 | 10417.98 | 3018135 | 0.003452 | | 1.734167 | 0.117 |
| | 1:11:25 | 71.41667 | 1.785417 | 903.13 | 0.28742 | 3142.196 | 300088 | 0.010471 | 4798.919 | 3018135 | 0.00159 | | 1.785417 | 0.066 |
| | 1:13:28 | 73.46667 | 1.836667 | 672.76 | 0.3089 | 2177.922 | 300088 | 0.007258 | 3326.231 | 3018135 | 0.001102 | | 1.836667 | 0.035 |
| | 1:15:31 | 75.51667 | 1.887917 | 505.23 | 0.2862 | 1765.304 | 300088 | 0.005883 | 2696.061 | 3018135 | 0.000893 | | 1.887917 | 0.017 |
| | 1:17:34 | 77.56667 | 1.939167 | 492.71 | 0.31507 | 1563.811 | 300088 | 0.005211 | 2388.331 | 3018135 | 0.000791 | | 1.939167 | 0.008 |
| | 1:19:37 | 79.61667 | 1.990417 | 439.92 | 0.29212 | 1505.956 | 300088 | 0.005018 | 2299.972 | 3018135 | 0.000762 | | 1.990417 | 0.004 |
| | 1:21:40 | 81.66667 | 2.041667 | 447.6 | 0.30832 | 1451.738 | 300088 | 0.004838 | 2217.168 | 3018135 | 0.000735 | | 2.041667 | 0.002 |
| | 1:23:43 | 83.71667 | 2.092917 | 464.71 | 0.32714 | 1420.523 | 300088 | 0.004734 | 2169.494 | 3018135 | 0.000719 | | 2.092917 | 0.001 |
| | 1:25:46 | 85.76667 | 2.144167 | 460.92 | 0.31857 | 1446.841 | 300088 | 0.004821 | 2209.687 | 3018135 | 0.000732 | | 2.144167 | 0 |
| | 1:27:49 | 87.81667 | 2.195417 | 420.91 | 0.2827 | 1488.893 | 300088 | 0.004962 | 2273.912 | 3018135 | 0.000753 | | 2.195417 | 0 |
| | 1:29:52 | 89.86667 | 2.246667 | 421.68 | 0.28468 | 1481.242 | 300088 | 0.004936 | 2262.227 | 3018135 | 0.00075 | | 2.246667 | 0 |
| | 1:31:55 | 91.91667 | 2.297917 | 410.25 | 0.2835 | 1447.09 | 300088 | 0.004822 | 2210.068 | 3018135 | 0.000732 | | 2.297917 | 0 |
| | 1:33:58 | 93.96667 | 2.349167 | 378.03 | 0.29724 | 1271.801 | 300088 | 0.004238 | 1942.357 | 3018135 | 0.000644 | | 2.349167 | 0 |
| | 1:36:01 | 96.01667 | 2.400417 | 335.41 | 0.2904 | 1154.993 | 300088 | 0.003849 | 1763.963 | 3018135 | 0.000584 | | 2.400417 | 0 |
| | 1:38:04 | 98.06667 | 2.451667 | 313.83 | 0.30426 | 1031.453 | 300088 | 0.003437 | 1575.287 | 3018135 | 0.000522 | | 2.451667 | 0 |
| | 1:40:07 | 100.1167 | 2.502917 | 282.31 | 0.2999 | 941.3471 | 300088 | 0.003137 | 1437.672 | 3018135 | 0.000476 | | 2.502917 | 0 |
| | | | | | | | | | | | | | | |
| | | | | | | | | | 3007956 | | 0.996627 | | | |

| 5/95% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:24:15 | 24.25 | 0.60625 | 24.28 | 0.27883 | 87.07815 | 336095 | 0.000259 | 132.9901 | 3087318 | 4.31E-05 | | 0.60625 | 0 |
| mobil. | 0:26:18 | 26.3 | 0.6575 | 76.9 | 0.31713 | 242.4873 | 336095 | 0.000721 | 370.3387 | 3087318 | 0.00012 | | 0.6575 | 0 |
| | 0:28:21 | 28.35 | 0.70875 | 189.93 | 0.30453 | 623.6824 | 336095 | 0.001856 | 952.5189 | 3087318 | 0.000309 | | 0.70875 | 0 |
| flow | 0:30:24 | 30.4 | 0.76 | 391.95 | 0.28275 | 1386.207 | 336095 | 0.004124 | 2117.084 | 3087318 | 0.000686 | | 0.76 | 0 |
| 0.745 | 0:32:27 | 32.45 | 0.81125 | 831.85 | 0.32269 | 2577.861 | 336095 | 0.00767 | 3937.038 | 3087318 | 0.001275 | | 0.81125 | 0 |
| (mL/min) | 0:34:30 | 34.5 | 0.8625 | 1239.13 | 0.27688 | 4475.332 | 336095 | 0.013316 | 6834.951 | 3087318 | 0.002214 | | 0.8625 | 0 |
| | 0:36:33 | 36.55 | 0.91375 | 2406.36 | 0.32824 | 7331.099 | 336095 | 0.021813 | 11196.42 | 3087318 | 0.003627 | | 0.91375 | 0 |
| | 0:38:36 | 38.6 | 0.965 | 3580.02 | 0.31534 | 11352.89 | 336095 | 0.033779 | 17338.7 | 3087318 | 0.005616 | | 0.965 | 0.001 |
| | 0:40:39 | 40.65 | 1.01625 | 4886.78 | 0.29164 | 16756.21 | 336095 | 0.049856 | 25590.92 | 3087318 | 0.008289 | | 1.01625 | 0.005 |
| | 0:42:42 | 42.7 | 1.0675 | 8406.34 | 0.31856 | 26388.56 | 336095 | 0.078515 | 40301.93 | 3087318 | 0.013054 | | 1.0675 | 0.025 |
| | 0:44:45 | 44.75 | 1.11875 | 13521.76 | 0.29005 | 46618.72 | 336095 | 0.138707 | 71198.44 | 3087318 | 0.023062 | | 1.11875 | 0.083 |
| | 0:46:48 | 46.8 | 1.17 | 20467.4 | 0.27096 | 75536.61 | 336095 | 0.224748 | 115363.3 | 3087318 | 0.037367 | | 1.17 | 0.202 |
| | 0:48:51 | 48.85 | 1.22125 | 34138 | 0.29446 | 115934.3 | 336095 | 0.344945 | 177060.6 | 3087318 | 0.057351 | | 1.22125 | 0.379 |
| | 0:50:54 | 50.9 | 1.2725 | 47216.34 | 0.27894 | 169270.6 | 336095 | 0.503639 | 258518.5 | 3087318 | 0.083736 | | 1.2725 | 0.582 |
| | 0:52:57 | 52.95 | 1.32375 | 74287.86 | 0.31499 | 235842 | 336095 | 0.701712 | 360189.6 | 3087318 | 0.116667 | | 1.32375 | 0.752 |
| | 0:55:00 | 55 | 1.375 | 82118.73 | 0.29904 | 274607.8 | 336095 | 0.817054 | 419394.8 | 3087318 | 0.135844 | | 1.375 | 0.854 |
| | 0:57:03 | 57.05 | 1.42625 | 69263.98 | 0.24783 | 279481.8 | 336095 | 0.831556 | 426838.6 | 3087318 | 0.138255 | | 1.42625 | 0.867 |
| | 0:59:06 | 59.1 | 1.4775 | 75311.37 | 0.28515 | 264111.4 | 336095 | 0.785824 | 403364.2 | 3087318 | 0.130652 | | 1.4775 | 0.781 |
| | 1:01:09 | 61.15 | 1.52875 | 53456.32 | 0.245 | 218189.1 | 336095 | 0.649189 | 333229.2 | 3087318 | 0.107935 | | 1.52875 | 0.618 |
| | 1:03:12 | 63.2 | 1.58 | 36521.73 | 0.27464 | 132980.4 | 336095 | 0.395663 | 203094.3 | 3087318 | 0.065783 | | 1.58 | 0.423 |
| | 1:05:15 | 65.25 | 1.63125 | 17111.88 | 0.30742 | 55662.87 | 336095 | 0.165616 | 85011.12 | 3087318 | 0.027536 | | 1.63125 | 0.249 |
| | 1:07:18 | 67.3 | 1.6825 | 5177.87 | 0.29538 | 17529.52 | 336095 | 0.052156 | 26771.96 | 3087318 | 0.008672 | | 1.6825 | 0.124 |
| | 1:09:21 | 69.35 | 1.73375 | 1895.02 | 0.28263 | 6704.95 | 336095 | 0.01995 | 10240.13 | 3087318 | 0.003317 | | 1.73375 | 0.054 |
| | 1:11:24 | 71.4 | 1.785 | 1087.8 | 0.29733 | 3658.561 | 336095 | 0.010885 | 5587.538 | 3087318 | 0.00181 | | 1.785 | 0.021 |
| | 1:13:27 | 73.45 | 1.83625 | 689.68 | 0.29112 | 2369.057 | 336095 | 0.007049 | 3618.143 | 3087318 | 0.001172 | | 1.83625 | 0.007 |
| | 1:15:30 | 75.5 | 1.8875 | 562.86 | 0.30316 | 1856.643 | 336095 | 0.005524 | 2835.559 | 3087318 | 0.000918 | | 1.8875 | 0.002 |
| | 1:17:33 | 77.55 | 1.93875 | 470.63 | 0.29837 | 1577.337 | 336095 | 0.004693 | 2408.988 | 3087318 | 0.00078 | | 1.93875 | 0.001 |
| | 1:19:36 | 79.6 | 1.99 | 419.41 | 0.30442 | 1377.735 | 336095 | 0.004099 | 2104.145 | 3087318 | 0.000682 | | 1.99 | 0 |
| | 1:21:39 | 81.65 | 2.04125 | 387.44 | 0.30309 | 1278.3 | 336095 | 0.003803 | 1952.284 | 3087318 | 0.000632 | | 2.04125 | 0 |
| | 1:23:42 | 83.7 | 2.0925 | 368.09 | 0.30218 | 1218.115 | 336095 | 0.003624 | 1860.366 | 3087318 | 0.000603 | | 2.0925 | 0 |
| | 1:25:45 | 85.75 | 2.14375 | 316.3 | 0.27866 | 1135.075 | 336095 | 0.003377 | 1733.543 | 3087318 | 0.000562 | | 2.14375 | 0 |
| | 1:27:48 | 87.8 | 2.195 | 319.53 | 0.29993 | 1065.349 | 336095 | 0.00317 | 1627.054 | 3087318 | 0.000527 | | 2.195 | 0 |
| | 1:29:51 | 89.85 | 2.24625 | 312.82 | 0.3021 | 1035.485 | 336095 | 0.003081 | 1581.444 | 3087318 | 0.000512 | | 2.24625 | 0 |
| | 1:31:54 | 91.9 | 2.2975 | 290.62 | 0.2975 | 976.8739 | 336095 | 0.002907 | 1491.931 | 3087318 | 0.000483 | | 2.2975 | 0 |
| | 1:33:57 | 93.95 | 2.34875 | 283.43 | 0.29978 | 945.46 | 336095 | 0.002813 | 1443.954 | 3087318 | 0.000468 | | 2.34875 | 0 |
| | 1:36:00 | 96 | 2.4 | 260.05 | 0.28789 | 903.2964 | 336095 | 0.002688 | 1379.559 | 3087318 | 0.000447 | | 2.4 | 0 |
| | 1:38:03 | 98.05 | 2.45125 | 277.52 | 0.31231 | 888.6043 | 336095 | 0.002644 | 1357.121 | 3087318 | 0.00044 | | 2.45125 | 0 |
| | 1:40:06 | 100.1 | 2.5025 | 252.21 | 0.28273 | 892.0525 | 336095 | 0.002654 | 1362.387 | 3087318 | 0.000441 | | 2.5025 | 0 |
| | 1:42:09 | 102.15 | 2.55375 | 248.98 | 0.29302 | 849.7031 | 336095 | 0.002528 | 1297.709 | 3087318 | 0.00042 | | 2.55375 | 0 |
| | 1:44:12 | 104.2 | 2.605 | 222.53 | 0.28211 | 788.8058 | 336095 | 0.002347 | 1204.704 | 3087318 | 0.00039 | | 2.605 | 0 |
| | | | | | | | | | | | | | | |
| | | | | | | | | | 3033894 | | 0.982696 | | | |

| 10/90% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:18:00 | 18 | 0.45 | 20.82 | 0.312 | 66.73077 | 330477 | 0.000202 | 101.9146 | 3158815 | 3.23E-05 | | 0.45 | 0 |
| mobil. | 0:20:03 | 20.05 | 0.50125 | 66.1 | 0.28055 | 235.6086 | 330477 | 0.000713 | 359.8333 | 3158815 | 0.000114 | | 0.50125 | 0 |
| | 0:22:06 | 22.1 | 0.5525 | 180.07 | 0.29523 | 609.9312 | 330477 | 0.001846 | 931.5175 | 3158815 | 0.000295 | | 0.5525 | 0 |
| flow | 0:24:09 | 24.15 | 0.60375 | 414.97 | 0.28286 | 1467.051 | 330477 | 0.004439 | 2240.553 | 3158815 | 0.000709 | | 0.60375 | 0 |
| 0.745 | 0:26:12 | 26.2 | 0.655 | 712.75 | 0.27981 | 2547.264 | 330477 | 0.007708 | 3890.309 | 3158815 | 0.001232 | | 0.655 | 0 |
| (mL/min) | 0:28:15 | 28.25 | 0.70625 | 1204.84 | 0.29849 | 4036.45 | 330477 | 0.012214 | 6164.668 | 3158815 | 0.001952 | | 0.70625 | 0 |
| | 0:30:18 | 30.3 | 0.7575 | 1825.59 | 0.3048 | 5989.469 | 330477 | 0.018124 | 9147.416 | 3158815 | 0.002896 | | 0.7575 | 0 |
| | 0:32:21 | 32.35 | 0.80875 | 2378.39 | 0.29789 | 7984.122 | 330477 | 0.024159 | 12193.75 | 3158815 | 0.00386 | | 0.80875 | 0 |
| | 0:34:24 | 34.4 | 0.86 | 3200.63 | 0.29549 | 10831.6 | 330477 | 0.032776 | 16542.56 | 3158815 | 0.005237 | | 0.86 | 0 |
| | 0:36:27 | 36.45 | 0.91125 | 3908.43 | 0.29122 | 13420.88 | 330477 | 0.040611 | 20497.05 | 3158815 | 0.006489 | | 0.91125 | 0 |
| | 0:38:30 | 38.5 | 0.9625 | 5288.54 | 0.31541 | 16767.19 | 330477 | 0.050736 | 25607.69 | 3158815 | 0.008107 | | 0.9625 | 0.001 |
| | 0:40:33 | 40.55 | 1.01375 | 6594.05 | 0.30275 | 21780.51 | 330477 | 0.065906 | 33264.29 | 3158815 | 0.010531 | | 1.01375 | 0.007 |
| | 0:42:36 | 42.6 | 1.065 | 8986.83 | 0.29121 | 30860.31 | 330477 | 0.093381 | 47131.4 | 3158815 | 0.014921 | | 1.065 | 0.03 |
| | 0:44:39 | 44.65 | 1.11625 | 14676.4 | 0.29163 | 50325.41 | 330477 | 0.152281 | 76859.49 | 3158815 | 0.024332 | | 1.11625 | 0.093 |
| | 0:46:42 | 46.7 | 1.1675 | 23135.38 | 0.30645 | 75494.8 | 330477 | 0.228442 | 115299.4 | 3158815 | 0.036501 | | 1.1675 | 0.215 |
| | 0:48:45 | 48.75 | 1.21875 | 34465.5 | 0.31956 | 107853 | 330477 | 0.326355 | 164718.5 | 3158815 | 0.052146 | | 1.21875 | 0.388 |
| | 0:50:48 | 50.8 | 1.27 | 48089.36 | 0.29097 | 165272.6 | 330477 | 0.500103 | 252412.5 | 3158815 | 0.079907 | | 1.27 | 0.578 |
| | 0:52:51 | 52.85 | 1.32125 | 65700.31 | 0.29191 | 225070.4 | 330477 | 0.681047 | 343738.8 | 3158815 | 0.108819 | | 1.32125 | 0.741 |
| | 0:54:54 | 54.9 | 1.3725 | 83744.12 | 0.3179 | 263429.1 | 330477 | 0.797118 | 402322.1 | 3158815 | 0.127365 | | 1.3725 | 0.845 |
| | 0:56:57 | 56.95 | 1.42375 | 78543.33 | 0.29254 | 268487.5 | 330477 | 0.812424 | 410047.5 | 3158815 | 0.129811 | | 1.42375 | 0.866 |
| | 0:59:00 | 59 | 1.475 | 79894.62 | 0.32219 | 247973.6 | 330477 | 0.750351 | 378717.7 | 3158815 | 0.119892 | | 1.475 | 0.796 |
| | 1:01:03 | 61.05 | 1.52625 | 57778.29 | 0.26668 | 216657.8 | 330477 | 0.655591 | 330890.6 | 3158815 | 0.104751 | | 1.52625 | 0.65 |
| | 1:03:06 | 63.1 | 1.5775 | 45634.57 | 0.29909 | 152578.1 | 330477 | 0.46169 | 233024.8 | 3158815 | 0.07377 | | 1.5775 | 0.463 |
| | 1:05:09 | 65.15 | 1.62875 | 22443.62 | 0.30594 | 73359.55 | 330477 | 0.221981 | 112038.4 | 3158815 | 0.035468 | | 1.62875 | 0.289 |
| | 1:07:12 | 67.2 | 1.68 | 7169.69 | 0.30186 | 23751.71 | 330477 | 0.071871 | 36274.79 | 3158815 | 0.011484 | | 1.68 | 0.158 |
| | 1:09:15 | 69.25 | 1.73125 | 2541 | 0.2887 | 8801.524 | 330477 | 0.026633 | 13442.13 | 3158815 | 0.004255 | | 1.73125 | 0.075 |
| | 1:11:18 | 71.3 | 1.7825 | 1389.84 | 0.30252 | 4594.209 | 330477 | 0.013902 | 7016.505 | 3158815 | 0.002221 | | 1.7825 | 0.031 |
| | 1:13:21 | 73.35 | 1.83375 | 860.88 | 0.27971 | 3077.759 | 330477 | 0.009313 | 4700.508 | 3158815 | 0.001488 | | 1.83375 | 0.012 |
| | 1:15:24 | 75.4 | 1.885 | 658.3 | 0.293 | 2246.758 | 330477 | 0.006799 | 3431.361 | 3158815 | 0.001086 | | 1.885 | 0.004 |
| | 1:17:27 | 77.45 | 1.93625 | 494.23 | 0.27682 | 1785.384 | 330477 | 0.005402 | 2726.728 | 3158815 | 0.000863 | | 1.93625 | 0.001 |
| | 1:19:30 | 79.5 | 1.9875 | 426.05 | 0.28455 | 1497.276 | 330477 | 0.004531 | 2286.715 | 3158815 | 0.000724 | | 1.9875 | 0 |
| | 1:21:33 | 81.55 | 2.03875 | 331.55 | 0.26365 | 1257.538 | 330477 | 0.003805 | 1920.576 | 3158815 | 0.000608 | | 2.03875 | 0 |
| | 1:23:36 | 83.6 | 2.09 | 335.24 | 0.3039 | 1103.126 | 330477 | 0.003338 | 1684.749 | 3158815 | 0.000533 | | 2.09 | 0 |
| | 1:25:39 | 85.65 | 2.14125 | 267.85 | 0.28101 | 953.1689 | 330477 | 0.002884 | 1455.727 | 3158815 | 0.000461 | | 2.14125 | 0 |
| | 1:27:42 | 87.7 | 2.1925 | 249.14 | 0.28749 | 866.6041 | 330477 | 0.002622 | 1323.521 | 3158815 | 0.000419 | | 2.1925 | 0 |
| | 1:29:45 | 89.75 | 2.24375 | 232.61 | 0.29245 | 795.3838 | 330477 | 0.002407 | 1214.75 | 3158815 | 0.000385 | | 2.24375 | 0 |
| | 1:31:48 | 91.8 | 2.295 | 207.08 | 0.28459 | 727.6433 | 330477 | 0.002202 | 1111.293 | 3158815 | 0.000352 | | 2.295 | 0 |
| | 1:33:51 | 93.85 | 2.34625 | 195.4 | 0.27682 | 705.8739 | 330477 | 0.002136 | 1078.046 | 3158815 | 0.000341 | | 2.34625 | 0 |
| | 1:35:54 | 95.9 | 2.3975 | 186.91 | 0.27841 | 671.348 | 330477 | 0.002031 | 1025.316 | 3158815 | 0.000325 | | 2.3975 | 0 |
| | 1:37:57 | 97.95 | 2.44875 | 175.27 | 0.28578 | 613.3039 | 330477 | 0.001856 | 936.6684 | 3158815 | 0.000297 | | 2.44875 | 0 |
| | | | | | | | | | 3079772 | | 0.974977 | | | |

| 20/80% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:19:20 | 19.33333 | 0.483333 | 1159.79 | 0.30853 | 3759.083 | 300000 | 0.01253 | 5741.06 | 2793750 | 0.002055 | | 0.483333 | 0 |
| mobil. | 0:21:23 | 21.38333 | 0.534583 | 1513.23 | 0.29359 | 5154.229 | 300000 | 0.017181 | 7871.796 | 2793750 | 0.002818 | | 0.534583 | 0 |
| | 0:23:26 | 23.43333 | 0.585833 | 2095.41 | 0.3165 | 6620.569 | 300000 | 0.022069 | 10111.26 | 2793750 | 0.003619 | | 0.585833 | 0 |
| flow | 0:25:29 | 25.48333 | 0.637083 | 2378.47 | 0.28774 | 8266.039 | 300000 | 0.027553 | 12624.31 | 2793750 | 0.004519 | | 0.637083 | 0 |
| 0.745 | 0:27:32 | 27.53333 | 0.688333 | 2676.66 | 0.27057 | 9892.671 | 300000 | 0.032976 | 15108.58 | 2793750 | 0.005408 | | 0.688333 | 0 |
| (mL/min) | 0:29:35 | 29.58333 | 0.739583 | 3739.89 | 0.33339 | 11217.76 | 300000 | 0.037393 | 17132.33 | 2793750 | 0.006132 | | 0.739583 | 0 |
| | 0:31:38 | 31.63333 | 0.790833 | 4259.09 | 0.31983 | 13316.73 | 300000 | 0.044389 | 20337.98 | 2793750 | 0.00728 | | 0.790833 | 0 |
| | 0:33:41 | 33.68333 | 0.842083 | 4358.84 | 0.28177 | 15469.5 | 300000 | 0.051565 | 23625.79 | 2793750 | 0.008457 | | 0.842083 | 0 |
| | 0:35:44 | 35.73333 | 0.893333 | 5789.58 | 0.31795 | 18209.09 | 300000 | 0.060697 | 27809.83 | 2793750 | 0.009954 | | 0.893333 | 0 |
| | 0:37:47 | 37.78333 | 0.944583 | 5454.69 | 0.24726 | 22060.54 | 300000 | 0.073535 | 33691.97 | 2793750 | 0.01206 | | 0.944583 | 0 |
| | 0:39:50 | 39.83333 | 0.995833 | 8374.59 | 0.3003 | 27887.41 | 300000 | 0.092958 | 42591.05 | 2793750 | 0.015245 | | 0.995833 | 0.003 |
| | 0:41:53 | 41.88333 | 1.047083 | 14147.11 | 0.31629 | 44728.29 | 300000 | 0.149094 | 68311.28 | 2793750 | 0.024451 | | 1.047083 | 0.018 |
| | 0:43:56 | 43.93333 | 1.098333 | 20908.17 | 0.30507 | 68535.65 | 300000 | 0.228452 | 104671.1 | 2793750 | 0.037466 | | 1.098333 | 0.07 |
| | 0:45:59 | 45.98333 | 1.149583 | 28003.02 | 0.29972 | 93430.6 | 300000 | 0.311435 | 142691.9 | 2793750 | 0.051075 | | 1.149583 | 0.189 |
| | 0:48:02 | 48.03333 | 1.200833 | 31910.67 | 0.29751 | 107259.2 | 300000 | 0.357531 | 163811.5 | 2793750 | 0.058635 | | 1.200833 | 0.373 |
| | 0:50:05 | 50.08333 | 1.252083 | 36777.21 | 0.25819 | 142442.4 | 300000 | 0.474808 | 217545.2 | 2793750 | 0.077869 | | 1.252083 | 0.583 |
| | 0:52:08 | 52.13333 | 1.303333 | 64668.21 | 0.32706 | 197725.8 | 300000 | 0.659086 | 301976.8 | 2793750 | 0.10809 | | 1.303333 | 0.762 |
| | 0:54:11 | 54.18333 | 1.354583 | 73093.53 | 0.29337 | 249151.3 | 300000 | 0.830504 | 380516.4 | 2793750 | 0.136203 | | 1.354583 | 0.874 |
| | 0:56:14 | 56.23333 | 1.405833 | 79287.77 | 0.30359 | 261167.3 | 300000 | 0.870558 | 398867.7 | 2793750 | 0.142771 | | 1.405833 | 0.893 |
| | 0:58:17 | 58.28333 | 1.457083 | 56759.66 | 0.2491 | 227858.9 | 300000 | 0.75953 | 347997.6 | 2793750 | 0.124563 | | 1.457083 | 0.813 |
| | 1:00:20 | 60.33333 | 1.508333 | 54031.66 | 0.27867 | 193891.2 | 300000 | 0.646304 | 296120.3 | 2793750 | 0.105994 | | 1.508333 | 0.647 |
| | 1:02:23 | 62.38333 | 1.559583 | 37734.93 | 0.2824 | 133622.3 | 300000 | 0.445408 | 204074.6 | 2793750 | 0.073047 | | 1.559583 | 0.436 |
| | 1:04:26 | 64.43333 | 1.610833 | 17971.22 | 0.26943 | 66700.89 | 300000 | 0.222336 | 101868.9 | 2793750 | 0.036463 | | 1.610833 | 0.251 |
| | 1:06:29 | 66.48333 | 1.662083 | 6774.78 | 0.28947 | 23404.08 | 300000 | 0.078014 | 35743.89 | 2793750 | 0.012794 | | 1.662083 | 0.122 |
| | 1:08:32 | 68.53333 | 1.713333 | 2783 | 0.27866 | 9987.081 | 300000 | 0.03329 | 15252.77 | 2793750 | 0.00546 | | 1.713333 | 0.05 |
| | 1:10:35 | 70.58333 | 1.764583 | 1606.5 | 0.26804 | 5993.508 | 300000 | 0.019978 | 9153.586 | 2793750 | 0.003276 | | 1.764583 | 0.017 |
| | 1:12:38 | 72.63333 | 1.815833 | 1262.35 | 0.29968 | 4212.326 | 300000 | 0.014041 | 6433.276 | 2793750 | 0.002303 | | 1.815833 | 0.005 |
| | 1:14:41 | 74.68333 | 1.867083 | 935.11 | 0.27976 | 3342.544 | 300000 | 0.011142 | 5104.9 | 2793750 | 0.001827 | | 1.867083 | 0.001 |
| | 1:16:44 | 76.73333 | 1.918333 | 808.11 | 0.29278 | 2760.127 | 300000 | 0.0092 | 4215.404 | 2793750 | 0.001509 | | 1.918333 | 0 |
| | 1:18:47 | 78.78333 | 1.969583 | 647.87 | 0.28958 | 2237.275 | 300000 | 0.007458 | 3416.878 | 2793750 | 0.001223 | | 1.969583 | 0 |
| | 1:20:50 | 80.83333 | 2.020833 | 600.37 | 0.27606 | 2174.781 | 300000 | 0.007249 | 3321.434 | 2793750 | 0.001189 | | 2.020833 | 0 |
| | 1:22:53 | 82.88333 | 2.072083 | 499.59 | 0.29517 | 1692.55 | 300000 | 0.005642 | 2584.947 | 2793750 | 0.000925 | | 2.072083 | 0 |
| | 1:24:56 | 84.93333 | 2.123333 | 446.45 | 0.28542 | 1564.186 | 300000 | 0.005214 | 2388.903 | 2793750 | 0.000855 | | 2.123333 | 0 |
| | 1:26:59 | 86.98333 | 2.174583 | 380.49 | 0.26874 | 1415.829 | 300000 | 0.004719 | 2162.325 | 2793750 | 0.000774 | | 2.174583 | 0 |
| | 1:29:02 | 89.03333 | 2.225833 | 399.37 | 0.29257 | 1365.041 | 300000 | 0.00455 | 2084.759 | 2793750 | 0.000746 | | 2.225833 | 0 |
| | 1:31:05 | 91.08333 | 2.277083 | 374.28 | 0.28596 | 1308.854 | 300000 | 0.004363 | 1998.948 | 2793750 | 0.000716 | | 2.277083 | 0 |
| | 1:33:08 | 93.13333 | 2.328333 | 404.18 | 0.31267 | 1292.673 | 300000 | 0.004309 | 1974.235 | 2793750 | 0.000707 | | 2.328333 | 0 |
| | 1:35:11 | 95.18333 | 2.379583 | 387.42 | 0.2906 | 1333.173 | 300000 | 0.004444 | 2036.088 | 2793750 | 0.000729 | | 2.379583 | 0 |
| | 1:37:14 | 97.23333 | 2.430833 | 371.45 | 0.289 | 1285.294 | 300000 | 0.004284 | 1962.965 | 2793750 | 0.000703 | | 2.430833 | 0 |
| | 1:39:17 | 99.28333 | 2.482083 | 327.79 | 0.27217 | 1204.358 | 300000 | 0.004015 | 1839.355 | 2793750 | 0.000658 | | 2.482083 | 0 |
| | | | | | | | | | | | | | | |
| | | | | | | | | | 3046774 | | 1.090568 | | | |

| 50/50% | time | conv. | pore vol. | dpm | diff | dpm/diff | Co | C/Co | M | Mo | M/Mo | | pore vol. | CFIT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| pce | 0:17:20 | 17.33333 | 0.433333 | 874.28 | 0.30698 | 2848.003 | 340533 | 0.008363 | 4349.613 | 3298062 | 0.001319 | | 0.433333 | 0 |
| mobil. | 0:19:23 | 19.38333 | 0.484583 | 1315.54 | 0.28404 | 4631.531 | 340533 | 0.013601 | 7073.505 | 3298062 | 0.002145 | | 0.484583 | 0 |
| | 0:21:26 | 21.43333 | 0.535833 | 1896.97 | 0.29132 | 6511.637 | 340533 | 0.019122 | 9944.897 | 3298062 | 0.003015 | | 0.535833 | 0 |
| flow | 0:23:29 | 23.48333 | 0.587083 | 2363.15 | 0.29264 | 8075.28 | 340533 | 0.023714 | 12332.97 | 3298062 | 0.003739 | | 0.587083 | 0 |
| 0.745 | 0:25:32 | 25.53333 | 0.638333 | 2859.65 | 0.28363 | 10082.33 | 340533 | 0.029607 | 15398.23 | 3298062 | 0.004669 | | 0.638333 | 0 |
| (mL/min) | 0:27:35 | 27.58333 | 0.689583 | 2931.23 | 0.24484 | 11972.02 | 340533 | 0.035157 | 18284.27 | 3298062 | 0.005544 | | 0.689583 | 0 |
| | 0:29:38 | 29.63333 | 0.740833 | 4133.06 | 0.31632 | 13066.07 | 340533 | 0.038369 | 19955.16 | 3298062 | 0.006051 | | 0.740833 | 0 |
| | 0:31:41 | 31.68333 | 0.792083 | 4081.07 | 0.26427 | 15442.8 | 340533 | 0.045349 | 23585.02 | 3298062 | 0.007151 | | 0.792083 | 0 |
| | 0:33:44 | 33.73333 | 0.843333 | 5179.37 | 0.29769 | 17398.54 | 340533 | 0.051092 | 26571.91 | 3298062 | 0.008057 | | 0.843333 | 0 |
| | 0:35:47 | 35.78333 | 0.894583 | 5323.75 | 0.20651 | 25779.62 | 340533 | 0.075704 | 39371.93 | 3298062 | 0.011938 | | 0.894583 | 0 |
| | 0:37:50 | 37.83333 | 0.945833 | 6887.87 | 0.29388 | 23437.7 | 340533 | 0.068827 | 35795.22 | 3298062 | 0.010853 | | 0.945833 | 0.002 |
| | 0:39:53 | 39.88333 | 0.997083 | 8218.45 | 0.26754 | 30718.58 | 340533 | 0.090207 | 46914.96 | 3298062 | 0.014225 | | 0.997083 | 0.011 |
| | 0:41:56 | 41.93333 | 1.048333 | 12478.23 | 0.28221 | 44216.12 | 340533 | 0.129844 | 67529.06 | 3298062 | 0.020475 | | 1.048333 | 0.038 |
| | 0:43:59 | 43.98333 | 1.099583 | 18074.86 | 0.26325 | 68660.44 | 340533 | 0.201626 | 104861.7 | 3298062 | 0.031795 | | 1.099583 | 0.103 |
| | 0:46:02 | 46.03333 | 1.150833 | 26627.14 | 0.28533 | 93320.51 | 340533 | 0.274042 | 142523.7 | 3298062 | 0.043214 | | 1.150833 | 0.215 |
| | 0:48:05 | 48.08333 | 1.202083 | 31560.02 | 0.27632 | 114215.5 | 340533 | 0.335402 | 174435.6 | 3298062 | 0.05289 | | 1.202083 | 0.37 |
| | 0:50:08 | 50.13333 | 1.253333 | 42102.3 | 0.29584 | 142314.4 | 340533 | 0.417917 | 217349.7 | 3298062 | 0.065902 | | 1.253333 | 0.541 |
| | 0:52:11 | 52.18333 | 1.304583 | 53185 | 0.26629 | 199725.9 | 340533 | 0.58651 | 305031.3 | 3298062 | 0.092488 | | 1.304583 | 0.698 |
| | 0:54:14 | 54.23333 | 1.355833 | 64220.88 | 0.23552 | 272677 | 340533 | 0.800736 | 416445.9 | 3298062 | 0.12627 | | 1.355833 | 0.801 |
| | 0:56:17 | 56.28333 | 1.407083 | 80991.62 | 0.26375 | 307077.2 | 340533 | 0.901755 | 468983.7 | 3298062 | 0.1422 | | 1.407083 | 0.835 |
| | 0:58:20 | 58.33333 | 1.458333 | 81131.92 | 0.27473 | 295315.1 | 340533 | 0.867214 | 451020 | 3298062 | 0.136753 | | 1.458333 | 0.788 |
| | 1:00:23 | 60.38333 | 1.509583 | 69519.22 | 0.27891 | 249253.2 | 340533 | 0.73195 | 380672 | 3298062 | 0.115423 | | 1.509583 | 0.669 |
| | 1:02:26 | 62.43333 | 1.560833 | 43099.63 | 0.2739 | 157355.3 | 340533 | 0.462085 | 240321 | 3298062 | 0.072867 | | 1.560833 | 0.511 |
| | 1:04:29 | 64.48333 | 1.612083 | 20457.33 | 0.25065 | 81617.12 | 340533 | 0.239675 | 124649.7 | 3298062 | 0.037795 | | 1.612083 | 0.349 |
| | 1:06:32 | 66.53333 | 1.663333 | 13732.04 | 0.28036 | 48980.03 | 340533 | 0.143833 | 74804.74 | 3298062 | 0.022681 | | 1.663333 | 0.214 |
| | 1:08:35 | 68.58333 | 1.714583 | 7758.49 | 0.27171 | 28554.3 | 340533 | 0.083852 | 43609.56 | 3298062 | 0.013223 | | 1.714583 | 0.116 |
| | 1:10:38 | 70.63333 | 1.765833 | 5318.8 | 0.25223 | 21087.1 | 340533 | 0.061924 | 32205.28 | 3298062 | 0.009765 | | 1.765833 | 0.058 |
| | 1:12:41 | 72.68333 | 1.817083 | 3995.84 | 0.25598 | 15609.97 | 340533 | 0.04584 | 23840.33 | 3298062 | 0.007229 | | 1.817083 | 0.026 |
| | 1:14:44 | 74.73333 | 1.868333 | 2685.7 | 0.26295 | 10213.73 | 340533 | 0.029993 | 15598.92 | 3298062 | 0.00473 | | 1.868333 | 0.011 |
| | 1:16:47 | 76.78333 | 1.919583 | 1747.7 | 0.26904 | 6496.06 | 340533 | 0.019076 | 9921.108 | 3298062 | 0.003008 | | 1.919583 | 0.004 |
| | 1:18:50 | 78.83333 | 1.970833 | 1079.37 | 0.25912 | 4165.522 | 340533 | 0.012232 | 6361.793 | 3298062 | 0.001929 | | 1.970833 | 0.001 |
| | 1:20:53 | 80.88333 | 2.022083 | 706.88 | 0.24885 | 2840.587 | 340533 | 0.008342 | 4338.286 | 3298062 | 0.001315 | | 2.022083 | 0 |
| | 1:22:56 | 82.93333 | 2.073333 | 530.9 | 0.27477 | 1932.161 | 340533 | 0.005674 | 2950.894 | 3298062 | 0.000895 | | 2.073333 | 0 |
| | 1:24:59 | 84.98333 | 2.124583 | 436.45 | 0.26683 | 1635.686 | 340533 | 0.004803 | 2498.101 | 3298062 | 0.000757 | | 2.124583 | 0 |
| | 1:27:02 | 87.03333 | 2.175833 | 343.78 | 0.25692 | 1338.082 | 340533 | 0.003929 | 2043.586 | 3298062 | 0.00062 | | 2.175833 | 0 |
| | 1:29:05 | 89.08333 | 2.227083 | 304.76 | 0.2656 | 1147.44 | 340533 | 0.00337 | 1752.427 | 3298062 | 0.000531 | | 2.227083 | 0 |
| | 1:31:08 | 91.13333 | 2.278333 | 263.51 | 0.25724 | 1024.374 | 340533 | 0.003008 | 1564.475 | 3298062 | 0.000474 | | 2.278333 | 0 |
| | 1:33:11 | 93.18333 | 2.329583 | 215.32 | 0.24725 | 870.8595 | 340533 | 0.002557 | 1330.02 | 3298062 | 0.000403 | | 2.329583 | 0 |
| | 1:35:14 | 95.23333 | 2.380833 | 204.73 | 0.24934 | 821.0877 | 340533 | 0.002411 | 1254.006 | 3298062 | 0.00038 | | 2.380833 | 0 |
| | 1:37:17 | 97.28333 | 2.432083 | 189.36 | 0.25113 | 754.0318 | 340533 | 0.002214 | 1151.595 | 3298062 | 0.000349 | | 2.432083 | 0 |
| | | | | | | | | | | | | | | |
| | | | | | | | | | 3578626 | | 1.085069 | | | |

# *Appendix B. CFITM Input Files*

```
    1
    2    1   25  40
  Methanol Run: 0% Methanol/100% Water
PECLET       RF           PULSE
      5.0         1.0      0.319
    1    1    0
     0.400  0.0000
     0.451  0.0000
     0.503  0.0000
     0.554  0.0000
     0.605  0.0000
     0.656  0.0000
     0.708  0.0000
     0.759  0.0000
     0.810  0.0000
     0.861  0.0000
     0.913  0.0000
     0.964  0.0028
     1.015  0.0111
     1.066  0.0184
     1.118  0.0320
     1.169  0.0563
     1.220  0.0911
     1.271  0.1527
     1.323  0.2566
     1.374  0.4205
     1.425  0.5675
     1.476  0.6260
     1.528  0.6289
     1.579  0.5736
     1.630  0.4732
     1.681  0.3275
     1.733  0.1455
     1.784  0.0284
     1.835  0.0000
     1.886  0.0000
     1.938  0.0000
     1.989  0.0000
     2.040  0.0000
     2.091  0.0000
     2.143  0.0000
     2.194  0.0000
     2.245  0.0000
     2.296  0.0000
     2.348  0.0000
     2.399  0.0000
C$stop
```

```
    1
    2    1   25  40
  Methanol Run: 1% Methanol/99% Water
PECLET        RF           PULSE
      5.0         1.0      0.326
    1    1     0
     0.431   0.0000
     0.483   0.0000
     0.534   0.0000
     0.585   0.0000
     0.636   0.0000
     0.688   0.0000
     0.739   0.0000
     0.790   0.0000
     0.841   0.0000
     0.893   0.0000
     0.944   0.0000
     0.995   0.0046
     1.046   0.0136
     1.098   0.0245
     1.149   0.0436
     1.200   0.0820
     1.251   0.1352
     1.303   0.2179
     1.354   0.3383
     1.405   0.4895
     1.456   0.6194
     1.508   0.6339
     1.559   0.6113
     1.610   0.5364
     1.661   0.4029
     1.713   0.2162
     1.764   0.0678
     1.815   0.0000
     1.866   0.0000
     1.918   0.0000
     1.969   0.0000
     2.020   0.0000
     2.071   0.0000
     2.123   0.0000
     2.174   0.0000
     2.225   0.0000
     2.276   0.0000
     2.328   0.0000
     2.379   0.0000
     2.430   0.0000
C$stop
```

```
    1
    2    .1    25   40
  Methanol Run: 5% Methanol/95% Water
PECLET        RF            PULSE
      5.0          1.0       0.326
    1     1     0
     0.456   0.0000
     0.508   0.0000
     0.559   0.0000
     0.610   0.0000
     0.661   0.0000
     0.713   0.0000
     0.764   0.0000
     0.815   0.0000
     0.866   0.0000
     0.918   0.0000
     0.969   0.0000
     1.020   0.0000
     1.071   0.0024
     1.123   0.0108
     1.174   0.0318
     1.225   0.0926
     1.276   0.2447
     1.328   0.4720
     1.379   0.6573
     1.430   0.7483
     1.481   0.7455
     1.533   0.7510
     1.584   0.6581
     1.635   0.4568
     1.686   0.1993
     1.738   0.0302
     1.789   0.0000
     1.840   0.0000
     1.891   0.0000
     1.943   0.0000
     1.994   0.0000
     2.045   0.0000
     2.096   0.0000
     2.148   0.0000
     2.199   0.0000
     2.250   0.0000
     2.301   0.0000
     2.353   0.0000
     2.404   0.0000
     2.455   0.0000
C$stop
```

```
    1
    2   . 1    25  40
  Methanol Run: 10% Methanol/90% Water
PECLET       RF          PULSE
      5.0        1.0      0.328
    1    1     0
     0.394   0.0000
     0.445   0.0000
     0.496   0.0000
     0.548   0.0000
     0.599   0.0000
     0.650   0.0000
     0.701   0.0000
     0.753   0.0000
     0.804   0.0000
     0.855   0.0000
     0.906   0.0000
     0.958   0.0000
     1.009   0.0000
     1.060   0.0018
     1.111   0.0041
     1.163   0.0353
     1.214   0.1728
     1.265   0.4012
     1.316   0.6129
     1.368   0.7223
     1.419   0.8058
     1.470   0.7435
     1.521   0.6161
     1.573   0.5071
     1.624   0.3088
     1.675   0.0880
     1.726   0.0000
     1.778   0.0000
     1.829   0.0000
     1.880   0.0000
     1.931   0.0000
     1.983   0.0000
     2.034   0.0000
     2.085   0.0000
     2.136   0.0000
     2.188   0.0000
     2.239   0.0000
     2.290   0.0000
     2.341   0.0000
     2.393   0.0000
C$stop
```

```
     1
     2    .1    25   40
  Methanol Run: 20% Methanol/80% Water
PECLET        RF            PULSE
       5.0          1.0       0.322
     1    1     0
      0.440   0.0000
      0.491   0.0000
      0.542   0.0000
      0.593   0.0000
      0.645   0.0000
      0.696   0.0000
      0.747   0.0000
      0.798   0.0000
      0.850   0.0000
      0.901   0.0000
      0.952   0.0000
      1.003   0.0000
      1.055   0.0017
      1.106   0.0017
      1.157   0.0043
      1.208   0.0173
      1.260   0.0605
      1.311   0.1710
      1.362   0.3301
      1.413   0.5278
      1.465   0.7038
      1.516   0.7881
      1.567   0.8223
      1.618   0.7540
      1.670   0.7254
      1.721   0.5936
      1.772   0.4118
      1.823   0.1756
      1.875   0.0421
      1.926   0.0000
      1.977   0.0000
      2.028   0.0000
      2.080   0.0000
      2.131   0.0000
      2.182   0.0000
      2.233   0.0000
      2.285   0.0000
      2.336   0.0000
      2.387   0.0000
      2.438   0.0000
C$stop
```

```
     1
     2   . 1    25  40
  Methanol Run: 50% Methanol/50% Water
PECLET        RF            PULSE
      5.0          1.0       0.331
     1    1     0
      0.406  0.0000
      0.458  0.0000
      0.509  0.0000
      0.560  0.0000
      0.611  0.0000
      0.663  0.0000
      0.714  0.0000
      0.765  0.0000
      0.816  0.0000
      0.868  0.0000
      0.919  0.0000
      0.970  0.0000
      1.021  0.0000
      1.073  0.0000
      1.124  0.0000
      1.175  0.0177
      1.226  0.0789
      1.278  0.2270
      1.329  0.3950
      1.380  0.6083
      1.431  0.7144
      1.483  0.7184
      1.534  0.7253
      1.585  0.7146
      1.636  0.6797
      1.688  0.5980
      1.739  0.4776
      1.790  0.2658
      1.841  0.0970
      1.893  0.0184
      1.944  0.0000
      1.995  0.0000
      2.046  0.0000
      2.098  0.0000
      2.149  0.0000
      2.200  0.0000
      2.251  0.0000
      2.303  0.0000
      2.354  0.0000
      2.405  0.0000
C$stop
```

```
     1
     2    .1    25   40
   PCE Run: 0% Methanol/100% Water
 PECLET        RF           PULSE
     159.          1.0       0.334
     0     1     0     0     0
      0.552   0.0000
      0.603   0.0000
      0.655   0.0000
      0.706   0.0000
      0.757   0.0000
      0.808   0.0000
      0.860   0.0000
      0.911   0.0000
      0.962   0.0005
      1.013   0.0021
      1.065   0.0084
      1.116   0.0597
      1.167   0.2889
      1.218   0.5989
      1.270   0.8106
      1.321   0.9129
      1.372   0.9490
      1.423   0.9235
      1.475   0.7407
      1.526   0.4700
      1.577   0.2397
      1.628   0.1175
      1.680   0.0521
      1.731   0.0261
      1.782   0.0160
      1.833   0.0123
      1.885   0.0103
      1.936   0.0089
      1.987   0.0078
      2.038   0.0067
      2.090   0.0058
      2.141   0.0048
      2.192   0.0036
      2.243   0.0028
      2.295   0.0022
      2.346   0.0017
      2.397   0.0013
      2.448   0.0011
      2.500   0.0010
      2.551   0.0008
C$stop
```

```
     1
     2    1   25  40
   PCE Run: 1% Methanol/99% Water
PECLET        RF            PULSE
     153.          1.0       0.337
     0    1     0
      0.504   0.0000
      0.555   0.0001
      0.607   0.0005
      0.658   0.0013
      0.709   0.0028
      0.760   0.0057
      0.812   0.0099
      0.863   0.0165
      0.914   0.0247
      0.965   0.0359
      1.017   0.0530
      1.068   0.0820
      1.119   0.1413
      1.170   0.2641
      1.222   0.4469
      1.273   0.6510
      1.324   0.8571
      1.375   0.8900
      1.427   0.8853
      1.478   0.7760
      1.529   0.6292
      1.580   0.4164
      1.632   0.2006
      1.683   0.0725
      1.734   0.0227
      1.785   0.0105
      1.837   0.0073
      1.888   0.0059
      1.939   0.0052
      1.990   0.0050
      2.042   0.0048
      2.093   0.0047
      2.144   0.0048
      2.195   0.0050
      2.247   0.0049
      2.298   0.0048
      2.349   0.0042
      2.400   0.0038
      2.452   0.0034
      2.503   0.0031
C$stop
```

```
     1
     2    1   25  40
   PCE Run: 5% Methanol/95% Water
 PECLET       RF          PULSE
     305.         1.0      0.309
     0    1     0
      0.606   0.0003
      0.658   0.0007
      0.709   0.0019
      0.760   0.0041
      0.811   0.0077
      0.863   0.0133
      0.914   0.0218
      0.965   0.0338
      1.016   0.0499
      1.068   0.0785
      1.119   0.1387
      1.170   0.2247
      1.221   0.3449
      1.273   0.5036
      1.324   0.7017
      1.375   0.8171
      1.426   0.8316
      1.478   0.7858
      1.529   0.6491
      1.580   0.3957
      1.631   0.1656
      1.683   0.0522
      1.734   0.0200
      1.785   0.0109
      1.836   0.0070
      1.888   0.0055
      1.939   0.0047
      1.990   0.0041
      2.041   0.0038
      2.093   0.0036
      2.144   0.0034
      2.195   0.0032
      2.246   0.0031
      2.298   0.0029
      2.349   0.0028
      2.400   0.0027
      2.451   0.0026
      2.503   0.0027
      2.554   0.0025
      2.605   0.0023
C$stop
```

```
    1
    2    1   25  40
  PCE Run: 10% Methanol/90% Water
PECLET       RF           PULSE
    276.          1.0      0.320
    0    1     0
     0.450  0.0002
     0.501  0.0007
     0.553  0.0018
     0.604  0.0044
     0.655  0.0077
     0.706  0.0122
     0.758  0.0181
     0.809  0.0242
     0.860  0.0328
     0.911  0.0406
     0.963  0.0507
     1.014  0.0659
     1.065  0.0934
     1.116  0.1523
     1.168  0.2284
     1.219  0.3264
     1.270  0.5001
     1.321  0.6810
     1.373  0.7971
     1.424  0.8124
     1.475  0.7504
     1.526  0.6556
     1.578  0.4617
     1.629  0.2220
     1.680  0.0719
     1.731  0.0266
     1.783  0.0139
     1.834  0.0093
     1.885  0.0068
     1.936  0.0054
     1.988  0.0045
     2.039  0.0038
     2.090  0.0033
     2.141  0.0029
     2.193  0.0026
     2.244  0.0024
     2.295  0.0022
     2.346  0.0021
     2.398  0.0020
     2.449  0.0019
C$stop
```

```
     1
     2    1   25  40
   PCE Run: 20% Methanol/80% Water
 PECLET       RF          PULSE
     328.         1.0      0.313
     0    1     0
      0.483  0.0125
      0.535  0.0172
      0.586  0.0221
      0.637  0.0276
      0.688  0.0330
      0.740  0.0374
      0.791  0.0444
      0.842  0.0516
      0.893  0.0607
      0.945  0.0735
      0.996  0.0930
      1.047  0.1491
      1.098  0.2285
      1.150  0.3114
      1.201  0.3575
      1.252  0.4748
      1.303  0.6591
      1.355  0.8305
      1.406  0.8706
      1.457  0.7595
      1.508  0.6463
      1.560  0.4454
      1.611  0.2223
      1.662  0.0708
      1.713  0.0333
      1.765  0.0120
      1.816  0.0140
      1.867  0.0111
      1.918  0.0092
      1.970  0.0075
      2.021  0.0072
      2.072  0.0056
      2.123  0.0052
      2.175  0.0047
      2.226  0.0046
      2.277  0.0044
      2.328  0.0043
      2.380  0.0044
      2.431  0.0043
      2.482  0.0040
C$stop
```

```
    1
    2    1   25  40
  PCE Run: 50% Methanol/50% Water
PECLET       RF           PULSE
    221.          1.0      0.326
    0    1     0
     0.433  0.0084
     0.485  0.0136
     0.536  0.0191
     0.587  0.0237
     0.638  0.0296
     0.690  0.0352
     0.741  0.0384
     0.792  0.0453
     0.843  0.0511
     0.895  0.0757
     0.946  0.0688
     0.997  0.0902
     1.048  0.1298
     1.100  0.2016
     1.151  0.2740
     1.202  0.3354
     1.253  0.4179
     1.305  0.5865
     1.356  0.8007
     1.407  0.9018
     1.458  0.8672
     1.510  0.7320
     1.561  0.4621
     1.612  0.2397
     1.663  0.1438
     1.715  0.0839
     1.766  0.0619
     1.817  0.0458
     1.868  0.0300
     1.920  0.0191
     1.971  0.0122
     2.022  0.0083
     2.073  0.0057
     2.125  0.0048
     2.176  0.0039
     2.227  0.0034
     2.278  0.0030
     2.330  0.0026
     2.381  0.0024
     2.432  0.0022
C$stop
```

# *Appendix C. CFITM Output Files*

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 0% Methanol/100% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.319 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4000 | 0.0000 |
| 2 | 0.4510 | 0.0000 |
| 3 | 0.5030 | 0.0000 |
| 4 | 0.5540 | 0.0000 |
| 5 | 0.6050 | 0.0000 |
| 6 | 0.6560 | 0.0000 |
| 7 | 0.7080 | 0.0000 |
| 8 | 0.7590 | 0.0000 |
| 9 | 0.8100 | 0.0000 |
| 10 | 0.8610 | 0.0000 |
| 11 | 0.9130 | 0.0000 |
| 12 | 0.9640 | 0.0028 |
| 13 | 1.0150 | 0.0111 |
| 14 | 1.0660 | 0.0184 |
| 15 | 1.1180 | 0.0320 |
| 16 | 1.1690 | 0.0563 |
| 17 | 1.2200 | 0.0911 |
| 18 | 1.2710 | 0.1527 |
| 19 | 1.3230 | 0.2566 |
| 20 | 1.3740 | 0.4205 |
| 21 | 1.4250 | 0.5675 |
| 22 | 1.4760 | 0.6260 |
| 23 | 1.5280 | 0.6289 |
| 24 | 1.5790 | 0.5736 |
| 25 | 1.6300 | 0.4732 |
| 26 | 1.6810 | 0.3275 |
| 27 | 1.7330 | 0.1455 |
| 28 | 1.7840 | 0.0284 |
| 29 | 1.8350 | 0.0000 |
| 30 | 1.8860 | 0.0000 |
| 31 | 1.9380 | 0.0000 |
| 32 | 1.9890 | 0.0000 |
| 33 | 2.0400 | 0.0000 |
| 34 | 2.0910 | 0.0000 |
| 35 | 2.1430 | 0.0000 |
| 36 | 2.1940 | 0.0000 |
| 37 | 2.2450 | 0.0000 |
| 38 | 2.2960 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.3480 | 0.0000 |
| 40 | 2.3990 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 1.7375172 | 5.00000 | 1.00000 |
| 1 | 1.3608561 | 3.95501 | 1.61202 |
| 2 | 1.1148545 | 10.48430 | 1.57499 |
| 3 | 0.9179355 | 21.69042 | 1.26549 |
| 4 | 0.6162016 | 39.98299 | 1.41942 |
| 5 | 0.4030838 | 66.54190 | 1.31392 |
| 6 | 0.2705094 | 100.95358 | 1.35637 |
| 7 | 0.2326818 | 130.64368 | 1.34381 |
| 8 | 0.2254175 | 148.79398 | 1.34595 |
| 9 | 0.2245778 | 156.06346 | 1.34598 |
| 10 | 0.2245075 | 158.40369 | 1.34605 |
| 11 | 0.2245041 | 159.08281 | 1.34607 |
| 12 | 0.2245041 | 159.09472 | 1.34607 |

CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0432 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 159.09472 | 23.1279 | 6.88 | 112.2719 | 205.9175 |
| 2 | RF | 1.34607 | 0.0110 | 122.14 | 1.3238 | 1.3684 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.400 | 0.000 | 0.000 | 0.000 | 13 | 1.015 | 0.011 | 0.006 | 0.005 |
| 2 | 0.451 | 0.000 | 0.000 | 0.000 | 12 | 0.964 | 0.003 | 0.001 | 0.001 |
| 3 | 0.503 | 0.000 | 0.000 | 0.000 | 14 | 1.066 | 0.018 | 0.018 | 0.000 |
| 4 | 0.554 | 0.000 | 0.000 | 0.000 | 1 | 0.400 | 0.000 | 0.000 | 0.000 |
| 5 | 0.605 | 0.000 | 0.000 | 0.000 | 2 | 0.451 | 0.000 | 0.000 | 0.000 |
| 6 | 0.656 | 0.000 | 0.000 | 0.000 | 3 | 0.503 | 0.000 | 0.000 | 0.000 |
| 7 | 0.708 | 0.000 | 0.000 | 0.000 | 4 | 0.554 | 0.000 | 0.000 | 0.000 |
| 8 | 0.759 | 0.000 | 0.000 | 0.000 | 5 | 0.605 | 0.000 | 0.000 | 0.000 |
| 9 | 0.810 | 0.000 | 0.000 | 0.000 | 6 | 0.656 | 0.000 | 0.000 | 0.000 |
| 10 | 0.861 | 0.000 | 0.000 | 0.000 | 7 | 0.708 | 0.000 | 0.000 | 0.000 |
| 11 | 0.913 | 0.000 | 0.000 | 0.000 | 8 | 0.759 | 0.000 | 0.000 | 0.000 |
| 12 | 0.964 | 0.003 | 0.001 | 0.001 | 9 | 0.810 | 0.000 | 0.000 | 0.000 |
| 13 | 1.015 | 0.011 | 0.006 | 0.005 | 10 | 0.861 | 0.000 | 0.000 | 0.000 |
| 14 | 1.066 | 0.018 | 0.018 | 0.000 | 40 | 2.399 | 0.000 | 0.000 | 0.000 |
| 15 | 1.118 | 0.032 | 0.048 | -0.016 | 39 | 2.348 | 0.000 | 0.000 | 0.000 |
| 16 | 1.169 | 0.056 | 0.103 | -0.047 | 11 | 0.913 | 0.000 | 0.000 | 0.000 |
| 17 | 1.220 | 0.091 | 0.189 | -0.098 | 38 | 2.296 | 0.000 | 0.000 | 0.000 |
| 18 | 1.271 | 0.153 | 0.303 | -0.150 | 37 | 2.245 | 0.000 | 0.001 | -0.001 |
| 19 | 1.323 | 0.257 | 0.434 | -0.178 | 36 | 2.194 | 0.000 | 0.001 | -0.001 |
| 20 | 1.374 | 0.420 | 0.558 | -0.138 | 35 | 2.143 | 0.000 | 0.003 | -0.003 |
| 21 | 1.425 | 0.568 | 0.656 | -0.088 | 34 | 2.091 | 0.000 | 0.007 | -0.007 |
| 22 | 1.476 | 0.626 | 0.708 | -0.082 | 33 | 2.040 | 0.000 | 0.014 | -0.014 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 23 | 1.528 | 0.629 | 0.704 | -0.075 | 15 | 1.118 | 0.032 | 0.048 | -0.016 |
| 24 | 1.579 | 0.574 | 0.646 | -0.073 | 32 | 1.989 | 0.000 | 0.026 | -0.026 |
| 25 | 1.630 | 0.473 | 0.550 | -0.077 | 16 | 1.169 | 0.056 | 0.103 | -0.047 |
| 26 | 1.681 | 0.328 | 0.435 | -0.108 | 31 | 1.938 | 0.000 | 0.049 | -0.049 |
| 27 | 1.733 | 0.145 | 0.318 | -0.173 | 24 | 1.579 | 0.574 | 0.646 | -0.073 |
| 28 | 1.784 | 0.028 | 0.219 | -0.190 | 23 | 1.528 | 0.629 | 0.704 | -0.075 |
| 29 | 1.835 | 0.000 | 0.141 | -0.141 | 25 | 1.630 | 0.473 | 0.550 | -0.077 |
| 30 | 1.886 | 0.000 | 0.086 | -0.086 | 22 | 1.476 | 0.626 | 0.708 | -0.082 |
| 31 | 1.938 | 0.000 | 0.049 | -0.049 | 30 | 1.886 | 0.000 | 0.086 | -0.086 |
| 32 | 1.989 | 0.000 | 0.026 | -0.026 | 21 | 1.425 | 0.568 | 0.656 | -0.088 |
| 33 | 2.040 | 0.000 | 0.014 | -0.014 | 17 | 1.220 | 0.091 | 0.189 | -0.098 |
| 34 | 2.091 | 0.000 | 0.007 | -0.007 | 26 | 1.681 | 0.328 | 0.435 | -0.108 |
| 35 | 2.143 | 0.000 | 0.003 | -0.003 | 20 | 1.374 | 0.420 | 0.558 | -0.138 |
| 36 | 2.194 | 0.000 | 0.001 | -0.001 | 29 | 1.835 | 0.000 | 0.141 | -0.141 |
| 37 | 2.245 | 0.000 | 0.001 | -0.001 | 18 | 1.271 | 0.153 | 0.303 | -0.150 |
| 38 | 2.296 | 0.000 | 0.000 | 0.000 | 27 | 1.733 | 0.145 | 0.318 | -0.173 |
| 39 | 2.348 | 0.000 | 0.000 | 0.000 | 19 | 1.323 | 0.257 | 0.434 | -0.178 |
| 40 | 2.399 | 0.000 | 0.000 | 0.000 | 28 | 1.784 | 0.028 | 0.219 | -0.190 |

END OF PROBLEM

1 **********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 1% Methanol/99% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.326 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4310 | 0.0000 |
| 2 | 0.4830 | 0.0000 |
| 3 | 0.5340 | 0.0000 |
| 4 | 0.5850 | 0.0000 |
| 5 | 0.6360 | 0.0000 |
| 6 | 0.6880 | 0.0000 |
| 7 | 0.7390 | 0.0000 |
| 8 | 0.7900 | 0.0000 |
| 9 | 0.8410 | 0.0000 |
| 10 | 0.8930 | 0.0000 |
| 11 | 0.9440 | 0.0000 |
| 12 | 0.9950 | 0.0046 |
| 13 | 1.0460 | 0.0136 |
| 14 | 1.0980 | 0.0245 |
| 15 | 1.1490 | 0.0436 |
| 16 | 1.2000 | 0.0820 |
| 17 | 1.2510 | 0.1352 |
| 18 | 1.3030 | 0.2179 |
| 19 | 1.3540 | 0.3383 |
| 20 | 1.4050 | 0.4895 |
| 21 | 1.4560 | 0.6194 |
| 22 | 1.5080 | 0.6339 |
| 23 | 1.5590 | 0.6113 |
| 24 | 1.6100 | 0.5364 |
| 25 | 1.6610 | 0.4029 |
| 26 | 1.7130 | 0.2162 |
| 27 | 1.7640 | 0.0678 |
| 28 | 1.8150 | 0.0000 |
| 29 | 1.8660 | 0.0000 |
| 30 | 1.9180 | 0.0000 |
| 31 | 1.9690 | 0.0000 |
| 32 | 2.0200 | 0.0000 |
| 33 | 2.0710 | 0.0000 |
| 34 | 2.1230 | 0.0000 |
| 35 | 2.1740 | 0.0000 |
| 36 | 2.2250 | 0.0000 |
| 37 | 2.2760 | 0.0000 |
| 38 | 2.3280 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.3790 | 0.0000 |
| 40 | 2.4300 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 1.7593414 | 5.00000 | 1.00000 |
| 1 | 1.3673960 | 4.02193 | 1.60697 |
| 2 | 1.1304704 | 10.36198 | 1.57879 |
| 3 | 0.9330030 | 20.88302 | 1.26978 |
| 4 | 0.6351175 | 38.60093 | 1.41651 |
| 5 | 0.4244203 | 63.76383 | 1.31535 |
| 6 | 0.2966283 | 96.48217 | 1.35419 |
| 7 | 0.2591371 | 124.63864 | 1.34265 |
| 8 | 0.2515045 | 142.14987 | 1.34461 |
| 9 | 0.2505274 | 149.52063 | 1.34467 |
| 10 | 0.2504351 | 152.03288 | 1.34476 |
| 11 | 0.2504297 | 152.80571 | 1.34478 |
| 12 | 0.2504297 | 152.83439 | 1.34478 |

1 CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0425 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 152.83439 | 23.2397 | 6.58 | 105.7853 | 199.8834 |
| 2 | RF | 1.34478 | 0.0117 | 114.60 | 1.3210 | 1.3685 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.431 | 0.000 | 0.000 | 0.000 | 12 | 0.995 | 0.005 | 0.004 | 0.001 |
| 2 | 0.483 | 0.000 | 0.000 | 0.000 | 13 | 1.046 | 0.014 | 0.014 | 0.000 |
| 3 | 0.534 | 0.000 | 0.000 | 0.000 | 1 | 0.431 | 0.000 | 0.000 | 0.000 |
| 4 | 0.585 | 0.000 | 0.000 | 0.000 | 2 | 0.483 | 0.000 | 0.000 | 0.000 |
| 5 | 0.636 | 0.000 | 0.000 | 0.000 | 3 | 0.534 | 0.000 | 0.000 | 0.000 |
| 6 | 0.688 | 0.000 | 0.000 | 0.000 | 4 | 0.585 | 0.000 | 0.000 | 0.000 |
| 7 | 0.739 | 0.000 | 0.000 | 0.000 | 5 | 0.636 | 0.000 | 0.000 | 0.000 |
| 8 | 0.790 | 0.000 | 0.000 | 0.000 | 6 | 0.688 | 0.000 | 0.000 | 0.000 |
| 9 | 0.841 | 0.000 | 0.000 | 0.000 | 7 | 0.739 | 0.000 | 0.000 | 0.000 |
| 10 | 0.893 | 0.000 | 0.000 | 0.000 | 8 | 0.790 | 0.000 | 0.000 | 0.000 |
| 11 | 0.944 | 0.000 | 0.001 | -0.001 | 9 | 0.841 | 0.000 | 0.000 | 0.000 |
| 12 | 0.995 | 0.005 | 0.004 | 0.001 | 40 | 2.430 | 0.000 | 0.000 | 0.000 |
| 13 | 1.046 | 0.014 | 0.014 | 0.000 | 39 | 2.379 | 0.000 | 0.000 | 0.000 |
| 14 | 1.098 | 0.025 | 0.037 | -0.013 | 10 | 0.893 | 0.000 | 0.000 | 0.000 |
| 15 | 1.149 | 0.044 | 0.084 | -0.040 | 38 | 2.328 | 0.000 | 0.000 | 0.000 |
| 16 | 1.200 | 0.082 | 0.159 | -0.077 | 37 | 2.276 | 0.000 | 0.001 | -0.001 |
| 17 | 1.251 | 0.135 | 0.262 | -0.127 | 11 | 0.944 | 0.000 | 0.001 | -0.001 |
| 18 | 1.303 | 0.218 | 0.388 | -0.170 | 36 | 2.225 | 0.000 | 0.001 | -0.001 |
| 19 | 1.354 | 0.338 | 0.515 | -0.176 | 35 | 2.174 | 0.000 | 0.003 | -0.003 |
| 20 | 1.405 | 0.489 | 0.623 | -0.133 | 34 | 2.123 | 0.000 | 0.005 | -0.005 |
| 21 | 1.456 | 0.619 | 0.694 | -0.074 | 33 | 2.071 | 0.000 | 0.011 | -0.011 |
| 22 | 1.508 | 0.634 | 0.714 | -0.080 | 14 | 1.098 | 0.025 | 0.037 | -0.013 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 23 | 1.559 | 0.611 | 0.680 | -0.068 | 32 | 2.020 | 0.000 | 0.021 | -0.021 |
| 24 | 1.610 | 0.536 | 0.601 | -0.064 | 31 | 1.969 | 0.000 | 0.039 | -0.039 |
| 25 | 1.661 | 0.403 | 0.494 | -0.091 | 15 | 1.149 | 0.044 | 0.084 | -0.040 |
| 26 | 1.713 | 0.216 | 0.377 | -0.160 | 24 | 1.610 | 0.536 | 0.601 | -0.064 |
| 27 | 1.764 | 0.068 | 0.270 | -0.202 | 23 | 1.559 | 0.611 | 0.680 | -0.068 |
| 28 | 1.815 | 0.000 | 0.182 | -0.182 | 30 | 1.918 | 0.000 | 0.068 | -0.068 |
| 29 | 1.866 | 0.000 | 0.115 | -0.115 | 21 | 1.456 | 0.619 | 0.694 | -0.074 |
| 30 | 1.918 | 0.000 | 0.068 | -0.068 | 16 | 1.200 | 0.082 | 0.159 | -0.077 |
| 31 | 1.969 | 0.000 | 0.039 | -0.039 | 22 | 1.508 | 0.634 | 0.714 | -0.080 |
| 32 | 2.020 | 0.000 | 0.021 | -0.021 | 25 | 1.661 | 0.403 | 0.494 | -0.091 |
| 33 | 2.071 | 0.000 | 0.011 | -0.011 | 29 | 1.866 | 0.000 | 0.115 | -0.115 |
| 34 | 2.123 | 0.000 | 0.005 | -0.005 | 17 | 1.251 | 0.135 | 0.262 | -0.127 |
| 35 | 2.174 | 0.000 | 0.003 | -0.003 | 20 | 1.405 | 0.489 | 0.623 | -0.133 |
| 36 | 2.225 | 0.000 | 0.001 | -0.001 | 26 | 1.713 | 0.216 | 0.377 | -0.160 |
| 37 | 2.276 | 0.000 | 0.001 | -0.001 | 18 | 1.303 | 0.218 | 0.388 | -0.170 |
| 38 | 2.328 | 0.000 | 0.000 | 0.000 | 19 | 1.354 | 0.338 | 0.515 | -0.176 |
| 39 | 2.379 | 0.000 | 0.000 | 0.000 | 28 | 1.815 | 0.000 | 0.182 | -0.182 |
| 40 | 2.430 | 0.000 | 0.000 | 0.000 | 27 | 1.764 | 0.068 | 0.270 | -0.202 |

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 5% Methanol/95% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.326 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4560 | 0.0000 |
| 2 | 0.5080 | 0.0000 |
| 3 | 0.5590 | 0.0000 |
| 4 | 0.6100 | 0.0000 |
| 5 | 0.6610 | 0.0000 |
| 6 | 0.7130 | 0.0000 |
| 7 | 0.7640 | 0.0000 |
| 8 | 0.8150 | 0.0000 |
| 9 | 0.8660 | 0.0000 |
| 10 | 0.9180 | 0.0000 |
| 11 | 0.9690 | 0.0000 |
| 12 | 1.0200 | 0.0000 |
| 13 | 1.0710 | 0.0024 |
| 14 | 1.1230 | 0.0108 |
| 15 | 1.1740 | 0.0318 |
| 16 | 1.2250 | 0.0926 |
| 17 | 1.2760 | 0.2447 |
| 18 | 1.3280 | 0.4720 |
| 19 | 1.3790 | 0.6573 |
| 20 | 1.4300 | 0.7483 |
| 21 | 1.4810 | 0.7455 |
| 22 | 1.5330 | 0.7510 |
| 23 | 1.5840 | 0.6581 |
| 24 | 1.6350 | 0.4568 |
| 25 | 1.6860 | 0.1993 |
| 26 | 1.7380 | 0.0302 |
| 27 | 1.7890 | 0.0000 |
| 28 | 1.8400 | 0.0000 |
| 29 | 1.8910 | 0.0000 |
| 30 | 1.9430 | 0.0000 |
| 31 | 1.9940 | 0.0000 |
| 32 | 2.0450 | 0.0000 |
| 33 | 2.0960 | 0.0000 |
| 34 | 2.1480 | 0.0000 |
| 35 | 2.1990 | 0.0000 |
| 36 | 2.2500 | 0.0000 |
| 37 | 2.3010 | 0.0000 |
| 38 | 2.3530 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.4040 | 0.0000 |
| 40 | 2.4550 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 2.5125510 | 5.00000 | 1.00000 |
| 1 | 2.0375895 | 6.02197 | 1.63007 |
| 2 | 1.8661717 | 16.81586 | 1.14096 |
| 3 | 1.3585833 | 28.57618 | 1.46650 |
| 4 | 1.2421442 | 55.70067 | 1.18348 |
| 5 | 0.6307918 | 77.18728 | 1.37174 |
| 6 | 0.3239347 | 132.13273 | 1.28056 |
| 7 | 0.1571142 | 206.50526 | 1.32136 |
| 8 | 0.1274750 | 264.84063 | 1.31176 |
| 9 | 0.1242359 | 294.52444 | 1.31329 |
| 10 | 0.1240597 | 302.77202 | 1.31336 |
| 11 | 0.1240537 | 304.56661 | 1.31339 |
| 12 | 0.1240537 | 304.74452 | 1.31339 |
| 13 | 0.1240537 | 304.75780 | 1.31339 |

1 CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0775 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 304.75780 | 39.7658 | 7.66 | 224.2514 | 385.2642 |
| 2 | RF | 1.31339 | 0.0059 | 220.81 | 1.3014 | 1.3254 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.456 | 0.000 | 0.000 | 0.000 | 1 | 0.456 | 0.000 | 0.000 | 0.000 |
| 2 | 0.508 | 0.000 | 0.000 | 0.000 | 2 | 0.508 | 0.000 | 0.000 | 0.000 |
| 3 | 0.559 | 0.000 | 0.000 | 0.000 | 3 | 0.559 | 0.000 | 0.000 | 0.000 |
| 4 | 0.610 | 0.000 | 0.000 | 0.000 | 4 | 0.610 | 0.000 | 0.000 | 0.000 |
| 5 | 0.661 | 0.000 | 0.000 | 0.000 | 5 | 0.661 | 0.000 | 0.000 | 0.000 |
| 6 | 0.713 | 0.000 | 0.000 | 0.000 | 6 | 0.713 | 0.000 | 0.000 | 0.000 |
| 7 | 0.764 | 0.000 | 0.000 | 0.000 | 7 | 0.764 | 0.000 | 0.000 | 0.000 |
| 8 | 0.815 | 0.000 | 0.000 | 0.000 | 40 | 2.455 | 0.000 | 0.000 | 0.000 |
| 9 | 0.866 | 0.000 | 0.000 | 0.000 | 8 | 0.815 | 0.000 | 0.000 | 0.000 |
| 10 | 0.918 | 0.000 | 0.000 | 0.000 | 39 | 2.404 | 0.000 | 0.000 | 0.000 |
| 11 | 0.969 | 0.000 | 0.000 | 0.000 | 38 | 2.353 | 0.000 | 0.000 | 0.000 |
| 12 | 1.020 | 0.000 | 0.001 | -0.001 | 9 | 0.866 | 0.000 | 0.000 | 0.000 |
| 13 | 1.071 | 0.002 | 0.006 | -0.003 | 37 | 2.301 | 0.000 | 0.000 | 0.000 |
| 14 | 1.123 | 0.011 | 0.026 | -0.015 | 36 | 2.250 | 0.000 | 0.000 | 0.000 |
| 15 | 1.174 | 0.032 | 0.083 | -0.051 | 10 | 0.918 | 0.000 | 0.000 | 0.000 |
| 16 | 1.225 | 0.093 | 0.194 | -0.102 | 35 | 2.199 | 0.000 | 0.000 | 0.000 |
| 17 | 1.276 | 0.245 | 0.360 | -0.116 | 34 | 2.148 | 0.000 | 0.000 | 0.000 |
| 18 | 1.328 | 0.472 | 0.554 | -0.082 | 11 | 0.969 | 0.000 | 0.000 | 0.000 |
| 19 | 1.379 | 0.657 | 0.724 | -0.066 | 33 | 2.096 | 0.000 | 0.000 | 0.000 |
| 20 | 1.430 | 0.748 | 0.838 | -0.090 | 32 | 2.045 | 0.000 | 0.000 | 0.000 |
| 21 | 1.481 | 0.746 | 0.875 | -0.130 | 12 | 1.020 | 0.000 | 0.001 | -0.001 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 22 | 1.533 | 0.751 | 0.824 | -0.073 | 31 | 1.994 | 0.000 | 0.002 | -0.002 |
| 23 | 1.584 | 0.658 | 0.693 | -0.035 | 13 | 1.071 | 0.002 | 0.006 | -0.003 |
| 24 | 1.635 | 0.457 | 0.513 | -0.056 | 30 | 1.943 | 0.000 | 0.005 | -0.005 |
| 25 | 1.686 | 0.199 | 0.332 | -0.133 | 29 | 1.891 | 0.000 | 0.015 | -0.015 |
| 26 | 1.738 | 0.030 | 0.185 | -0.155 | 14 | 1.123 | 0.011 | 0.026 | -0.015 |
| 27 | 1.789 | 0.000 | 0.091 | -0.091 | 23 | 1.584 | 0.658 | 0.693 | -0.035 |
| 28 | 1.840 | 0.000 | 0.039 | -0.039 | 28 | 1.840 | 0.000 | 0.039 | -0.039 |
| 29 | 1.891 | 0.000 | 0.015 | -0.015 | 15 | 1.174 | 0.032 | 0.083 | -0.051 |
| 30 | 1.943 | 0.000 | 0.005 | -0.005 | 24 | 1.635 | 0.457 | 0.513 | -0.056 |
| 31 | 1.994 | 0.000 | 0.002 | -0.002 | 19 | 1.379 | 0.657 | 0.724 | -0.066 |
| 32 | 2.045 | 0.000 | 0.000 | 0.000 | 22 | 1.533 | 0.751 | 0.824 | -0.073 |
| 33 | 2.096 | 0.000 | 0.000 | 0.000 | 18 | 1.328 | 0.472 | 0.554 | -0.082 |
| 34 | 2.148 | 0.000 | 0.000 | 0.000 | 20 | 1.430 | 0.748 | 0.838 | -0.090 |
| 35 | 2.199 | 0.000 | 0.000 | 0.000 | 27 | 1.789 | 0.000 | 0.091 | -0.091 |
| 36 | 2.250 | 0.000 | 0.000 | 0.000 | 16 | 1.225 | 0.093 | 0.194 | -0.102 |
| 37 | 2.301 | 0.000 | 0.000 | 0.000 | 17 | 1.276 | 0.245 | 0.360 | -0.116 |
| 38 | 2.353 | 0.000 | 0.000 | 0.000 | 21 | 1.481 | 0.746 | 0.875 | -0.130 |
| 39 | 2.404 | 0.000 | 0.000 | 0.000 | 25 | 1.686 | 0.199 | 0.332 | -0.133 |
| 40 | 2.455 | 0.000 | 0.000 | 0.000 | 26 | 1.738 | 0.030 | 0.185 | -0.155 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 10% Methanol/90% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.328 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.3940 | 0.0000 |
| 2 | 0.4450 | 0.0000 |
| 3 | 0.4960 | 0.0000 |
| 4 | 0.5480 | 0.0000 |
| 5 | 0.5990 | 0.0000 |
| 6 | 0.6500 | 0.0000 |
| 7 | 0.7010 | 0.0000 |
| 8 | 0.7530 | 0.0000 |
| 9 | 0.8040 | 0.0000 |
| 10 | 0.8550 | 0.0000 |
| 11 | 0.9060 | 0.0000 |
| 12 | 0.9580 | 0.0000 |
| 13 | 1.0090 | 0.0000 |
| 14 | 1.0600 | 0.0018 |
| 15 | 1.1110 | 0.0041 |
| 16 | 1.1630 | 0.0353 |
| 17 | 1.2140 | 0.1728 |
| 18 | 1.2650 | 0.4012 |
| 19 | 1.3160 | 0.6129 |
| 20 | 1.3680 | 0.7223 |
| 21 | 1.4190 | 0.8058 |
| 22 | 1.4700 | 0.7435 |
| 23 | 1.5210 | 0.6161 |
| 24 | 1.5730 | 0.5071 |
| 25 | 1.6240 | 0.3088 |
| 26 | 1.6750 | 0.0880 |
| 27 | 1.7260 | 0.0000 |
| 28 | 1.7780 | 0.0000 |
| 29 | 1.8290 | 0.0000 |
| 30 | 1.8800 | 0.0000 |
| 31 | 1.9310 | 0.0000 |
| 32 | 1.9830 | 0.0000 |
| 33 | 2.0340 | 0.0000 |
| 34 | 2.0850 | 0.0000 |
| 35 | 2.1360 | 0.0000 |
| 36 | 2.1880 | 0.0000 |
| 37 | 2.2390 | 0.0000 |
| 38 | 2.2900 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.3410 | 0.0000 |
| 40 | 2.3930 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 2.3998257 | 5.00000 | 1.00000 |
| 1 | 1.9379348 | 6.79970 | 1.57860 |
| 2 | 1.8858709 | 17.65172 | 1.07969 |
| 3 | 1.3257426 | 25.74722 | 1.40975 |
| 4 | 1.1300019 | 52.26530 | 1.15333 |
| 5 | 0.5767929 | 80.24640 | 1.32332 |
| 6 | 0.2952515 | 129.93195 | 1.23941 |
| 7 | 0.1622297 | 199.68445 | 1.27236 |
| 8 | 0.1413681 | 247.17486 | 1.26468 |
| 9 | 0.1394053 | 269.29171 | 1.26545 |
| 10 | 0.1393203 | 274.57353 | 1.26543 |
| 11 | 0.1393184 | 275.58952 | 1.26542 |
| 12 | 0.1393184 | 275.61210 | 1.26542 |

1 CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0764 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 275.61210 | 37.8166 | 7.29 | 199.0518 | 352.1724 |
| 2 | RF | 1.26542 | 0.0064 | 199.14 | 1.2526 | 1.2783 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.394 | 0.000 | 0.000 | 0.000 | 1 | 0.394 | 0.000 | 0.000 | 0.000 |
| 2 | 0.445 | 0.000 | 0.000 | 0.000 | 2 | 0.445 | 0.000 | 0.000 | 0.000 |
| 3 | 0.496 | 0.000 | 0.000 | 0.000 | 3 | 0.496 | 0.000 | 0.000 | 0.000 |
| 4 | 0.548 | 0.000 | 0.000 | 0.000 | 4 | 0.548 | 0.000 | 0.000 | 0.000 |
| 5 | 0.599 | 0.000 | 0.000 | 0.000 | 5 | 0.599 | 0.000 | 0.000 | 0.000 |
| 6 | 0.650 | 0.000 | 0.000 | 0.000 | 6 | 0.650 | 0.000 | 0.000 | 0.000 |
| 7 | 0.701 | 0.000 | 0.000 | 0.000 | 7 | 0.701 | 0.000 | 0.000 | 0.000 |
| 8 | 0.753 | 0.000 | 0.000 | 0.000 | 8 | 0.753 | 0.000 | 0.000 | 0.000 |
| 9 | 0.804 | 0.000 | 0.000 | 0.000 | 40 | 2.393 | 0.000 | 0.000 | 0.000 |
| 10 | 0.855 | 0.000 | 0.000 | 0.000 | 39 | 2.341 | 0.000 | 0.000 | 0.000 |
| 11 | 0.906 | 0.000 | 0.000 | 0.000 | 9 | 0.804 | 0.000 | 0.000 | 0.000 |
| 12 | 0.958 | 0.000 | 0.001 | -0.001 | 38 | 2.290 | 0.000 | 0.000 | 0.000 |
| 13 | 1.009 | 0.000 | 0.004 | -0.004 | 37 | 2.239 | 0.000 | 0.000 | 0.000 |
| 14 | 1.060 | 0.002 | 0.018 | -0.017 | 10 | 0.855 | 0.000 | 0.000 | 0.000 |
| 15 | 1.111 | 0.004 | 0.063 | -0.059 | 36 | 2.188 | 0.000 | 0.000 | 0.000 |
| 16 | 1.163 | 0.035 | 0.160 | -0.125 | 35 | 2.136 | 0.000 | 0.000 | 0.000 |
| 17 | 1.214 | 0.173 | 0.313 | -0.140 | 11 | 0.906 | 0.000 | 0.000 | 0.000 |
| 18 | 1.265 | 0.401 | 0.498 | -0.097 | 34 | 2.085 | 0.000 | 0.000 | 0.000 |
| 19 | 1.316 | 0.613 | 0.676 | -0.063 | 33 | 2.034 | 0.000 | 0.000 | 0.000 |
| 20 | 1.368 | 0.722 | 0.810 | -0.088 | 12 | 0.958 | 0.000 | 0.001 | -0.001 |
| 21 | 1.419 | 0.806 | 0.871 | -0.065 | 32 | 1.983 | 0.000 | 0.001 | -0.001 |
| 22 | 1.470 | 0.744 | 0.848 | -0.104 | 31 | 1.931 | 0.000 | 0.003 | -0.003 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 23 | 1.521 | 0.616 | 0.741 | -0.125 | 13 | 1.009 | 0.000 | 0.004 | -0.004 |
| 24 | 1.573 | 0.507 | 0.571 | -0.064 | 30 | 1.880 | 0.000 | 0.008 | -0.008 |
| 25 | 1.624 | 0.309 | 0.388 | -0.079 | 14 | 1.060 | 0.002 | 0.018 | -0.017 |
| 26 | 1.675 | 0.088 | 0.231 | -0.143 | 29 | 1.829 | 0.000 | 0.022 | -0.022 |
| 27 | 1.726 | 0.000 | 0.120 | -0.120 | 28 | 1.778 | 0.000 | 0.055 | -0.055 |
| 28 | 1.778 | 0.000 | 0.055 | -0.055 | 15 | 1.111 | 0.004 | 0.063 | -0.059 |
| 29 | 1.829 | 0.000 | 0.022 | -0.022 | 19 | 1.316 | 0.613 | 0.676 | -0.063 |
| 30 | 1.880 | 0.000 | 0.008 | -0.008 | 24 | 1.573 | 0.507 | 0.571 | -0.064 |
| 31 | 1.931 | 0.000 | 0.003 | -0.003 | 21 | 1.419 | 0.806 | 0.871 | -0.065 |
| 32 | 1.983 | 0.000 | 0.001 | -0.001 | 25 | 1.624 | 0.309 | 0.388 | -0.079 |
| 33 | 2.034 | 0.000 | 0.000 | 0.000 | 20 | 1.368 | 0.722 | 0.810 | -0.088 |
| 34 | 2.085 | 0.000 | 0.000 | 0.000 | 18 | 1.265 | 0.401 | 0.498 | -0.097 |
| 35 | 2.136 | 0.000 | 0.000 | 0.000 | 22 | 1.470 | 0.744 | 0.848 | -0.104 |
| 36 | 2.188 | 0.000 | 0.000 | 0.000 | 27 | 1.726 | 0.000 | 0.120 | -0.120 |
| 37 | 2.239 | 0.000 | 0.000 | 0.000 | 23 | 1.521 | 0.616 | 0.741 | -0.125 |
| 38 | 2.290 | 0.000 | 0.000 | 0.000 | 16 | 1.163 | 0.035 | 0.160 | -0.125 |
| 39 | 2.341 | 0.000 | 0.000 | 0.000 | 17 | 1.214 | 0.173 | 0.313 | -0.140 |
| 40 | 2.393 | 0.000 | 0.000 | 0.000 | 26 | 1.675 | 0.088 | 0.231 | -0.143 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 20% Methanol/80% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.322 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4400 | 0.0000 |
| 2 | 0.4910 | 0.0000 |
| 3 | 0.5420 | 0.0000 |
| 4 | 0.5930 | 0.0000 |
| 5 | 0.6450 | 0.0000 |
| 6 | 0.6960 | 0.0000 |
| 7 | 0.7470 | 0.0000 |
| 8 | 0.7980 | 0.0000 |
| 9 | 0.8500 | 0.0000 |
| 10 | 0.9010 | 0.0000 |
| 11 | 0.9520 | 0.0000 |
| 12 | 1.0030 | 0.0000 |
| 13 | 1.0550 | 0.0017 |
| 14 | 1.1060 | 0.0017 |
| 15 | 1.1570 | 0.0043 |
| 16 | 1.2080 | 0.0173 |
| 17 | 1.2600 | 0.0605 |
| 18 | 1.3110 | 0.1710 |
| 19 | 1.3620 | 0.3301 |
| 20 | 1.4130 | 0.5278 |
| 21 | 1.4650 | 0.7038 |
| 22 | 1.5160 | 0.7881 |
| 23 | 1.5670 | 0.8223 |
| 24 | 1.6180 | 0.7540 |
| 25 | 1.6700 | 0.7254 |
| 26 | 1.7210 | 0.5936 |
| 27 | 1.7720 | 0.4118 |
| 28 | 1.8230 | 0.1756 |
| 29 | 1.8750 | 0.0421 |
| 30 | 1.9260 | 0.0000 |
| 31 | 1.9770 | 0.0000 |
| 32 | 2.0280 | 0.0000 |
| 33 | 2.0800 | 0.0000 |
| 34 | 2.1310 | 0.0000 |
| 35 | 2.1820 | 0.0000 |
| 36 | 2.2330 | 0.0000 |
| 37 | 2.2850 | 0.0000 |
| 38 | 2.3360 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.3870 | 0.0000 |
| 40 | 2.4380 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 3.1821863 | 5.00000 | 1.00000 |
| 1 | 2.6683041 | 4.62117 | 1.76768 |
| 2 | 2.1786787 | 11.35423 | 1.40497 |
| 3 | 1.2182719 | 37.32405 | 1.44531 |
| 4 | 0.4977078 | 103.62416 | 1.35778 |
| 5 | 0.1255254 | 198.04523 | 1.43351 |
| 6 | 0.0311304 | 282.26962 | 1.40335 |
| 7 | 0.0222684 | 323.83838 | 1.41066 |
| 8 | 0.0222296 | 328.22786 | 1.41062 |
| 9 | 0.0222295 | 328.24006 | 1.41065 |

1 CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0764 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 328.24006 | 17.6087 | 18.64 | 292.5910 | 363.8891 |
| 2 | RF | 1.41065 | 0.0026 | 543.86 | 1.4054 | 1.4159 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.440 | 0.000 | 0.000 | 0.000 | 26 | 1.721 | 0.594 | 0.537 | 0.057 |
| 2 | 0.491 | 0.000 | 0.000 | 0.000 | 27 | 1.772 | 0.412 | 0.360 | 0.051 |
| 3 | 0.542 | 0.000 | 0.000 | 0.000 | 21 | 1.465 | 0.704 | 0.683 | 0.021 |
| 4 | 0.593 | 0.000 | 0.000 | 0.000 | 25 | 1.670 | 0.725 | 0.705 | 0.020 |
| 5 | 0.645 | 0.000 | 0.000 | 0.000 | 20 | 1.413 | 0.528 | 0.508 | 0.020 |
| 6 | 0.696 | 0.000 | 0.000 | 0.000 | 19 | 1.362 | 0.330 | 0.326 | 0.004 |
| 7 | 0.747 | 0.000 | 0.000 | 0.000 | 13 | 1.055 | 0.002 | 0.000 | 0.002 |
| 8 | 0.798 | 0.000 | 0.000 | 0.000 | 14 | 1.106 | 0.002 | 0.001 | 0.001 |
| 9 | 0.850 | 0.000 | 0.000 | 0.000 | 1 | 0.440 | 0.000 | 0.000 | 0.000 |
| 10 | 0.901 | 0.000 | 0.000 | 0.000 | 2 | 0.491 | 0.000 | 0.000 | 0.000 |
| 11 | 0.952 | 0.000 | 0.000 | 0.000 | 3 | 0.542 | 0.000 | 0.000 | 0.000 |
| 12 | 1.003 | 0.000 | 0.000 | 0.000 | 4 | 0.593 | 0.000 | 0.000 | 0.000 |
| 13 | 1.055 | 0.002 | 0.000 | 0.002 | 5 | 0.645 | 0.000 | 0.000 | 0.000 |
| 14 | 1.106 | 0.002 | 0.001 | 0.001 | 6 | 0.696 | 0.000 | 0.000 | 0.000 |
| 15 | 1.157 | 0.004 | 0.005 | -0.001 | 7 | 0.747 | 0.000 | 0.000 | 0.000 |
| 16 | 1.208 | 0.017 | 0.023 | -0.006 | 8 | 0.798 | 0.000 | 0.000 | 0.000 |
| 17 | 1.260 | 0.060 | 0.074 | -0.013 | 9 | 0.850 | 0.000 | 0.000 | 0.000 |
| 18 | 1.311 | 0.171 | 0.174 | -0.003 | 10 | 0.901 | 0.000 | 0.000 | 0.000 |
| 19 | 1.362 | 0.330 | 0.326 | 0.004 | 40 | 2.438 | 0.000 | 0.000 | 0.000 |
| 20 | 1.413 | 0.528 | 0.508 | 0.020 | 11 | 0.952 | 0.000 | 0.000 | 0.000 |
| 21 | 1.465 | 0.704 | 0.683 | 0.021 | 39 | 2.387 | 0.000 | 0.000 | 0.000 |
| 22 | 1.516 | 0.788 | 0.806 | -0.018 | 38 | 2.336 | 0.000 | 0.000 | 0.000 |
| 23 | 1.567 | 0.822 | 0.857 | -0.035 | 12 | 1.003 | 0.000 | 0.000 | 0.000 |
| 24 | 1.618 | 0.754 | 0.823 | -0.069 | 37 | 2.285 | 0.000 | 0.000 | 0.000 |
| 25 | 1.670 | 0.725 | 0.705 | 0.020 | 36 | 2.233 | 0.000 | 0.000 | 0.000 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 26 | 1.721 | 0.594 | 0.537 | 0.057 | 35 | 2.182 | 0.000 | 0.000 | 0.000 |
| 27 | 1.772 | 0.412 | 0.360 | 0.051 | 34 | 2.131 | 0.000 | 0.001 | -0.001 |
| 28 | 1.823 | 0.176 | 0.212 | -0.037 | 15 | 1.157 | 0.004 | 0.005 | -0.001 |
| 29 | 1.875 | 0.042 | 0.109 | -0.066 | 33 | 2.080 | 0.000 | 0.002 | -0.002 |
| 30 | 1.926 | 0.000 | 0.050 | -0.050 | 18 | 1.311 | 0.171 | 0.174 | -0.003 |
| 31 | 1.977 | 0.000 | 0.020 | -0.020 | 16 | 1.208 | 0.017 | 0.023 | -0.006 |
| 32 | 2.028 | 0.000 | 0.007 | -0.007 | 32 | 2.028 | 0.000 | 0.007 | -0.007 |
| 33 | 2.080 | 0.000 | 0.002 | -0.002 | 17 | 1.260 | 0.060 | 0.074 | -0.013 |
| 34 | 2.131 | 0.000 | 0.001 | -0.001 | 22 | 1.516 | 0.788 | 0.806 | -0.018 |
| 35 | 2.182 | 0.000 | 0.000 | 0.000 | 31 | 1.977 | 0.000 | 0.020 | -0.020 |
| 36 | 2.233 | 0.000 | 0.000 | 0.000 | 23 | 1.567 | 0.822 | 0.857 | -0.035 |
| 37 | 2.285 | 0.000 | 0.000 | 0.000 | 28 | 1.823 | 0.176 | 0.212 | -0.037 |
| 38 | 2.336 | 0.000 | 0.000 | 0.000 | 30 | 1.926 | 0.000 | 0.050 | -0.050 |
| 39 | 2.387 | 0.000 | 0.000 | 0.000 | 29 | 1.875 | 0.042 | 0.109 | -0.066 |
| 40 | 2.438 | 0.000 | 0.000 | 0.000 | 24 | 1.618 | 0.754 | 0.823 | -0.069 |

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
Methanol Run: 50% Methanol/50% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 5.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.331 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4060 | 0.0000 |
| 2 | 0.4580 | 0.0000 |
| 3 | 0.5090 | 0.0000 |
| 4 | 0.5600 | 0.0000 |
| 5 | 0.6110 | 0.0000 |
| 6 | 0.6630 | 0.0000 |
| 7 | 0.7140 | 0.0000 |
| 8 | 0.7650 | 0.0000 |
| 9 | 0.8160 | 0.0000 |
| 10 | 0.8680 | 0.0000 |
| 11 | 0.9190 | 0.0000 |
| 12 | 0.9700 | 0.0000 |
| 13 | 1.0210 | 0.0000 |
| 14 | 1.0730 | 0.0000 |
| 15 | 1.1240 | 0.0000 |
| 16 | 1.1750 | 0.0177 |
| 17 | 1.2260 | 0.0789 |
| 18 | 1.2780 | 0.2270 |
| 19 | 1.3290 | 0.3950 |
| 20 | 1.3800 | 0.6083 |
| 21 | 1.4310 | 0.7144 |
| 22 | 1.4830 | 0.7184 |
| 23 | 1.5340 | 0.7253 |
| 24 | 1.5850 | 0.7146 |
| 25 | 1.6360 | 0.6797 |
| 26 | 1.6880 | 0.5980 |
| 27 | 1.7390 | 0.4776 |
| 28 | 1.7900 | 0.2658 |
| 29 | 1.8410 | 0.0970 |
| 30 | 1.8930 | 0.0184 |
| 31 | 1.9440 | 0.0000 |
| 32 | 1.9950 | 0.0000 |
| 33 | 2.0460 | 0.0000 |
| 34 | 2.0980 | 0.0000 |
| 35 | 2.1490 | 0.0000 |
| 36 | 2.2000 | 0.0000 |
| 37 | 2.2510 | 0.0000 |
| 38 | 2.3030 | 0.0000 |

| | | |
|---|---|---|
| 39 | 2.3540 | 0.0000 |
| 40 | 2.4050 | 0.0000 |

| ITERATION | SSQ | PECLET | RF |
|---|---|---|---|
| 0 | 2.9583570 | 5.00000 | 1.00000 |
| 1 | 2.3833102 | 5.80803 | 1.73222 |
| 2 | 1.8883046 | 13.34307 | 1.30709 |
| 3 | 1.0679509 | 39.74408 | 1.47595 |
| 4 | 0.9037115 | 91.46498 | 1.25007 |
| 5 | 0.2358949 | 114.46765 | 1.40446 |
| 6 | 0.0712604 | 182.02134 | 1.35552 |
| 7 | 0.0467000 | 218.05743 | 1.37170 |
| 8 | 0.0465927 | 221.29075 | 1.37083 |
| 9 | 0.0465926 | 221.15155 | 1.37086 |
| 10 | 0.0465926 | 221.15960 | 1.37086 |

1 CORRELATION MATRIX

| | 1 | 2 |
|---|---|---|
| 1 | 1.0000 | |
| 2 | 0.0615 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | PECLET | 221.15960 | 15.5099 | 14.26 | 189.7597 | 252.5595 |
| 2 | RF | 1.37086 | 0.0043 | 319.91 | 1.3622 | 1.3795 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.406 | 0.000 | 0.000 | 0.000 | 27 | 1.739 | 0.478 | 0.383 | 0.094 |
| 2 | 0.458 | 0.000 | 0.000 | 0.000 | 20 | 1.380 | 0.608 | 0.525 | 0.083 |
| 3 | 0.509 | 0.000 | 0.000 | 0.000 | 26 | 1.688 | 0.598 | 0.529 | 0.069 |
| 4 | 0.560 | 0.000 | 0.000 | 0.000 | 21 | 1.431 | 0.714 | 0.664 | 0.050 |
| 5 | 0.611 | 0.000 | 0.000 | 0.000 | 19 | 1.329 | 0.395 | 0.371 | 0.024 |
| 6 | 0.663 | 0.000 | 0.000 | 0.000 | 25 | 1.636 | 0.680 | 0.667 | 0.013 |
| 7 | 0.714 | 0.000 | 0.000 | 0.000 | 28 | 1.790 | 0.266 | 0.253 | 0.012 |
| 8 | 0.765 | 0.000 | 0.000 | 0.000 | 1 | 0.406 | 0.000 | 0.000 | 0.000 |
| 9 | 0.816 | 0.000 | 0.000 | 0.000 | 2 | 0.458 | 0.000 | 0.000 | 0.000 |
| 10 | 0.868 | 0.000 | 0.000 | 0.000 | 3 | 0.509 | 0.000 | 0.000 | 0.000 |
| 11 | 0.919 | 0.000 | 0.000 | 0.000 | 4 | 0.560 | 0.000 | 0.000 | 0.000 |
| 12 | 0.970 | 0.000 | 0.000 | 0.000 | 5 | 0.611 | 0.000 | 0.000 | 0.000 |
| 13 | 1.021 | 0.000 | 0.001 | -0.001 | 6 | 0.663 | 0.000 | 0.000 | 0.000 |
| 14 | 1.073 | 0.000 | 0.005 | -0.005 | 7 | 0.714 | 0.000 | 0.000 | 0.000 |
| 15 | 1.124 | 0.000 | 0.018 | -0.018 | 8 | 0.765 | 0.000 | 0.000 | 0.000 |
| 16 | 1.175 | 0.018 | 0.052 | -0.034 | 9 | 0.816 | 0.000 | 0.000 | 0.000 |
| 17 | 1.226 | 0.079 | 0.119 | -0.041 | 10 | 0.868 | 0.000 | 0.000 | 0.000 |
| 18 | 1.278 | 0.227 | 0.230 | -0.003 | 40 | 2.405 | 0.000 | 0.000 | 0.000 |
| 19 | 1.329 | 0.395 | 0.371 | 0.024 | 11 | 0.919 | 0.000 | 0.000 | 0.000 |
| 20 | 1.380 | 0.608 | 0.525 | 0.083 | 39 | 2.354 | 0.000 | 0.000 | 0.000 |
| 21 | 1.431 | 0.714 | 0.664 | 0.050 | 38 | 2.303 | 0.000 | 0.000 | 0.000 |
| 22 | 1.483 | 0.718 | 0.763 | -0.045 | 12 | 0.970 | 0.000 | 0.000 | 0.000 |
| 23 | 1.534 | 0.725 | 0.798 | -0.073 | 37 | 2.251 | 0.000 | 0.000 | 0.000 |
| 24 | 1.585 | 0.715 | 0.763 | -0.049 | 36 | 2.200 | 0.000 | 0.001 | -0.001 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 25 | 1.636 | 0.680 | 0.667 | 0.013 | 13 | 1.021 | 0.000 | 0.001 | -0.001 |
| 26 | 1.688 | 0.598 | 0.529 | 0.069 | 35 | 2.149 | 0.000 | 0.001 | -0.001 |
| 27 | 1.739 | 0.478 | 0.383 | 0.094 | 18 | 1.278 | 0.227 | 0.230 | -0.003 |
| 28 | 1.790 | 0.266 | 0.253 | 0.012 | 34 | 2.098 | 0.000 | 0.004 | -0.004 |
| 29 | 1.841 | 0.097 | 0.153 | -0.056 | 14 | 1.073 | 0.000 | 0.005 | -0.005 |
| 30 | 1.893 | 0.018 | 0.084 | -0.066 | 33 | 2.046 | 0.000 | 0.009 | -0.009 |
| 31 | 1.944 | 0.000 | 0.043 | -0.043 | 15 | 1.124 | 0.000 | 0.018 | -0.018 |
| 32 | 1.995 | 0.000 | 0.020 | -0.020 | 32 | 1.995 | 0.000 | 0.020 | -0.020 |
| 33 | 2.046 | 0.000 | 0.009 | -0.009 | 16 | 1.175 | 0.018 | 0.052 | -0.034 |
| 34 | 2.098 | 0.000 | 0.004 | -0.004 | 17 | 1.226 | 0.079 | 0.119 | -0.041 |
| 35 | 2.149 | 0.000 | 0.001 | -0.001 | 31 | 1.944 | 0.000 | 0.043 | -0.043 |
| 36 | 2.200 | 0.000 | 0.001 | -0.001 | 22 | 1.483 | 0.718 | 0.763 | -0.045 |
| 37 | 2.251 | 0.000 | 0.000 | 0.000 | 24 | 1.585 | 0.715 | 0.763 | -0.049 |
| 38 | 2.303 | 0.000 | 0.000 | 0.000 | 29 | 1.841 | 0.097 | 0.153 | -0.056 |
| 39 | 2.354 | 0.000 | 0.000 | 0.000 | 30 | 1.893 | 0.018 | 0.084 | -0.066 |
| 40 | 2.405 | 0.000 | 0.000 | 0.000 | 23 | 1.534 | 0.725 | 0.798 | -0.073 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 0% Methanol/100% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 159.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.334 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.5520 | 0.0000 |
| 2 | 0.6030 | 0.0000 |
| 3 | 0.6550 | 0.0000 |
| 4 | 0.7060 | 0.0000 |
| 5 | 0.7570 | 0.0000 |
| 6 | 0.8080 | 0.0000 |
| 7 | 0.8600 | 0.0000 |
| 8 | 0.9110 | 0.0000 |
| 9 | 0.9620 | 0.0005 |
| 10 | 1.0130 | 0.0021 |
| 11 | 1.0650 | 0.0084 |
| 12 | 1.1160 | 0.0597 |
| 13 | 1.1670 | 0.2889 |
| 14 | 1.2180 | 0.5989 |
| 15 | 1.2700 | 0.8106 |
| 16 | 1.3210 | 0.9129 |
| 17 | 1.3720 | 0.9490 |
| 18 | 1.4230 | 0.9235 |
| 19 | 1.4750 | 0.7407 |
| 20 | 1.5260 | 0.4700 |
| 21 | 1.5770 | 0.2397 |
| 22 | 1.6280 | 0.1175 |
| 23 | 1.6800 | 0.0521 |
| 24 | 1.7310 | 0.0261 |
| 25 | 1.7820 | 0.0160 |
| 26 | 1.8330 | 0.0123 |
| 27 | 1.8850 | 0.0103 |
| 28 | 1.9360 | 0.0089 |
| 29 | 1.9870 | 0.0078 |
| 30 | 2.0380 | 0.0067 |
| 31 | 2.0900 | 0.0058 |
| 32 | 2.1410 | 0.0048 |
| 33 | 2.1920 | 0.0036 |
| 34 | 2.2430 | 0.0028 |
| 35 | 2.2950 | 0.0022 |
| 36 | 2.3460 | 0.0017 |
| 37 | 2.3970 | 0.0013 |
| 38 | 2.4480 | 0.0011 |

| | |
|---|---|
| 39 | 2.5000 |
| 40 | 2.5510 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 3.5356415 | 1.00000 |
| 1 | 0.3227643 | 1.16641 |
| 2 | 0.2397820 | 1.20674 |
| 3 | 0.2355492 | 1.19223 |
| 4 | 0.2327444 | 1.19765 |
| 5 | 0.2327444 | 1.19765 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.19765 | 0.0097 | 124.03 | 1.1781 | 1.2172 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | RESI- OBS. | FITTED | DUAL | PORE NO | CONCENTRATION VOLUME | RESI- OBS. | FITTED | DUAL |
| 1 | 0.552 | 0.000 | 0.000 | 0.000 | 18 | 1.423 | 0.923 | 0.741 | 0.182 |
| 2 | 0.603 | 0.000 | 0.000 | 0.000 | 17 | 1.372 | 0.949 | 0.788 | 0.161 |
| 3 | 0.655 | 0.000 | 0.000 | 0.000 | 16 | 1.321 | 0.913 | 0.768 | 0.145 |
| 4 | 0.706 | 0.000 | 0.000 | 0.000 | 15 | 1.270 | 0.811 | 0.686 | 0.124 |
| 5 | 0.757 | 0.000 | 0.000 | 0.000 | 19 | 1.475 | 0.741 | 0.637 | 0.104 |
| 6 | 0.808 | 0.000 | 0.000 | 0.000 | 14 | 1.218 | 0.599 | 0.557 | 0.042 |
| 7 | 0.860 | 0.000 | 0.001 | -0.001 | 30 | 2.038 | 0.007 | 0.001 | 0.006 |
| 8 | 0.911 | 0.000 | 0.007 | -0.007 | 29 | 1.987 | 0.008 | 0.002 | 0.006 |
| 9 | 0.962 | 0.001 | 0.025 | -0.024 | 31 | 2.090 | 0.006 | 0.000 | 0.006 |
| 10 | 1.013 | 0.002 | 0.067 | -0.065 | 32 | 2.141 | 0.005 | 0.000 | 0.005 |
| 11 | 1.065 | 0.008 | 0.147 | -0.138 | 28 | 1.936 | 0.009 | 0.005 | 0.004 |
| 12 | 1.116 | 0.060 | 0.264 | -0.204 | 33 | 2.192 | 0.004 | 0.000 | 0.004 |
| 13 | 1.167 | 0.289 | 0.408 | -0.119 | 34 | 2.243 | 0.003 | 0.000 | 0.003 |
| 14 | 1.218 | 0.599 | 0.557 | 0.042 | 35 | 2.295 | 0.002 | 0.000 | 0.002 |
| 15 | 1.270 | 0.811 | 0.686 | 0.124 | 36 | 2.346 | 0.002 | 0.000 | 0.002 |
| 16 | 1.321 | 0.913 | 0.768 | 0.145 | 37 | 2.397 | 0.001 | 0.000 | 0.001 |
| 17 | 1.372 | 0.949 | 0.788 | 0.161 | 38 | 2.448 | 0.001 | 0.000 | 0.001 |
| 18 | 1.423 | 0.923 | 0.741 | 0.182 | 39 | 2.500 | 0.001 | 0.000 | 0.001 |
| 19 | 1.475 | 0.741 | 0.637 | 0.104 | 40 | 2.551 | 0.001 | 0.000 | 0.001 |
| 20 | 1.526 | 0.470 | 0.502 | -0.032 | 27 | 1.885 | 0.010 | 0.010 | 0.000 |
| 21 | 1.577 | 0.240 | 0.363 | -0.123 | 1 | 0.552 | 0.000 | 0.000 | 0.000 |
| 22 | 1.628 | 0.117 | 0.242 | -0.124 | 2 | 0.603 | 0.000 | 0.000 | 0.000 |
| 23 | 1.680 | 0.052 | 0.147 | -0.095 | 3 | 0.655 | 0.000 | 0.000 | 0.000 |
| 24 | 1.731 | 0.026 | 0.084 | -0.058 | 4 | 0.706 | 0.000 | 0.000 | 0.000 |
| 25 | 1.782 | 0.016 | 0.044 | -0.028 | 5 | 0.757 | 0.000 | 0.000 | 0.000 |
| 26 | 1.833 | 0.012 | 0.022 | -0.010 | 6 | 0.808 | 0.000 | 0.000 | 0.000 |
| 27 | 1.885 | 0.010 | 0.010 | 0.000 | 7 | 0.860 | 0.000 | 0.001 | -0.001 |
| 28 | 1.936 | 0.009 | 0.005 | 0.004 | 8 | 0.911 | 0.000 | 0.007 | -0.007 |
| 29 | 1.987 | 0.008 | 0.002 | 0.006 | 26 | 1.833 | 0.012 | 0.022 | -0.010 |
| 30 | 2.038 | 0.007 | 0.001 | 0.006 | 9 | 0.962 | 0.001 | 0.025 | -0.024 |
| 31 | 2.090 | 0.006 | 0.000 | 0.006 | 25 | 1.782 | 0.016 | 0.044 | -0.028 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 2.141 | 0.005 | 0.000 | 0.005 | 20 | 1.526 | 0.470 | 0.502 | -0.032 |
| 33 | 2.192 | 0.004 | 0.000 | 0.004 | 24 | 1.731 | 0.026 | 0.084 | -0.058 |
| 34 | 2.243 | 0.003 | 0.000 | 0.003 | 10 | 1.013 | 0.002 | 0.067 | -0.065 |
| 35 | 2.295 | 0.002 | 0.000 | 0.002 | 23 | 1.680 | 0.052 | 0.147 | -0.095 |
| 36 | 2.346 | 0.002 | 0.000 | 0.002 | 13 | 1.167 | 0.289 | 0.408 | -0.119 |
| 37 | 2.397 | 0.001 | 0.000 | 0.001 | 21 | 1.577 | 0.240 | 0.363 | -0.123 |
| 38 | 2.448 | 0.001 | 0.000 | 0.001 | 22 | 1.628 | 0.117 | 0.242 | -0.124 |
| 39 | 2.500 | 0.001 | 0.000 | 0.001 | 11 | 1.065 | 0.008 | 0.147 | -0.138 |
| 40 | 2.551 | 0.001 | 0.000 | 0.001 | 12 | 1.116 | 0.060 | 0.264 | -0.204 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 1% Methanol/99% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 153.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.337 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.5040 | 0.0000 |
| 2 | 0.5550 | 0.0001 |
| 3 | 0.6070 | 0.0005 |
| 4 | 0.6580 | 0.0013 |
| 5 | 0.7090 | 0.0028 |
| 6 | 0.7600 | 0.0057 |
| 7 | 0.8120 | 0.0099 |
| 8 | 0.8630 | 0.0165 |
| 9 | 0.9140 | 0.0247 |
| 10 | 0.9650 | 0.0359 |
| 11 | 1.0170 | 0.0530 |
| 12 | 1.0680 | 0.0820 |
| 13 | 1.1190 | 0.1413 |
| 14 | 1.1700 | 0.2641 |
| 15 | 1.2220 | 0.4469 |
| 16 | 1.2730 | 0.6510 |
| 17 | 1.3240 | 0.8571 |
| 18 | 1.3750 | 0.8900 |
| 19 | 1.4270 | 0.8853 |
| 20 | 1.4780 | 0.7760 |
| 21 | 1.5290 | 0.6292 |
| 22 | 1.5800 | 0.4164 |
| 23 | 1.6320 | 0.2006 |
| 24 | 1.6830 | 0.0725 |
| 25 | 1.7340 | 0.0227 |
| 26 | 1.7850 | 0.0105 |
| 27 | 1.8370 | 0.0073 |
| 28 | 1.8880 | 0.0059 |
| 29 | 1.9390 | 0.0052 |
| 30 | 1.9900 | 0.0050 |
| 31 | 2.0420 | 0.0048 |
| 32 | 2.0930 | 0.0047 |
| 33 | 2.1440 | 0.0048 |
| 34 | 2.1950 | 0.0050 |
| 35 | 2.2470 | 0.0049 |
| 36 | 2.2980 | 0.0048 |
| 37 | 2.3490 | 0.0042 |
| 38 | 2.4000 | 0.0038 |

| | | |
|---|---|---|
| 39 | 2.4520 | 0.0034 |
| 40 | 2.5030 | 0.0031 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 3.5295768 | 1.00000 |
| 1 | 0.4832896 | 1.15290 |
| 2 | 0.1273274 | 1.23162 |
| 3 | 0.1200646 | 1.21627 |
| 4 | 0.1184520 | 1.22041 |
| 5 | 0.1184520 | 1.22041 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.22041 | 0.0071 | 171.67 | 1.2060 | 1.2348 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | RESI- OBS. | FITTED | DUAL | PORE NO | CONCENTRATION VOLUME | RESI- OBS. | FITTED | DUAL |
| 1 | 0.504 | 0.000 | 0.000 | 0.000 | 19 | 1.427 | 0.885 | 0.755 | 0.131 |
| 2 | 0.555 | 0.000 | 0.000 | 0.000 | 17 | 1.324 | 0.857 | 0.732 | 0.125 |
| 3 | 0.607 | 0.001 | 0.000 | 0.000 | 18 | 1.375 | 0.890 | 0.775 | 0.115 |
| 4 | 0.658 | 0.001 | 0.000 | 0.001 | 20 | 1.478 | 0.776 | 0.676 | 0.100 |
| 5 | 0.709 | 0.003 | 0.000 | 0.003 | 21 | 1.529 | 0.629 | 0.558 | 0.071 |
| 6 | 0.760 | 0.006 | 0.000 | 0.006 | 9 | 0.914 | 0.025 | 0.005 | 0.019 |
| 7 | 0.812 | 0.010 | 0.000 | 0.010 | 16 | 1.273 | 0.651 | 0.634 | 0.017 |
| 8 | 0.863 | 0.017 | 0.001 | 0.015 | 10 | 0.965 | 0.036 | 0.019 | 0.016 |
| 9 | 0.914 | 0.025 | 0.005 | 0.019 | 8 | 0.863 | 0.017 | 0.001 | 0.015 |
| 10 | 0.965 | 0.036 | 0.019 | 0.016 | 7 | 0.812 | 0.010 | 0.000 | 0.010 |
| 11 | 1.017 | 0.053 | 0.055 | -0.002 | 6 | 0.760 | 0.006 | 0.000 | 0.006 |
| 12 | 1.068 | 0.082 | 0.121 | -0.039 | 34 | 2.195 | 0.005 | 0.000 | 0.005 |
| 13 | 1.119 | 0.141 | 0.223 | -0.082 | 35 | 2.247 | 0.005 | 0.000 | 0.005 |
| 14 | 1.170 | 0.264 | 0.355 | -0.091 | 36 | 2.298 | 0.005 | 0.000 | 0.005 |
| 15 | 1.222 | 0.447 | 0.502 | -0.055 | 33 | 2.144 | 0.005 | 0.000 | 0.005 |
| 16 | 1.273 | 0.651 | 0.634 | 0.017 | 37 | 2.349 | 0.004 | 0.000 | 0.004 |
| 17 | 1.324 | 0.857 | 0.732 | 0.125 | 32 | 2.093 | 0.005 | 0.001 | 0.004 |
| 18 | 1.375 | 0.890 | 0.775 | 0.115 | 38 | 2.400 | 0.004 | 0.000 | 0.004 |
| 19 | 1.427 | 0.885 | 0.755 | 0.131 | 39 | 2.452 | 0.003 | 0.000 | 0.003 |
| 20 | 1.478 | 0.776 | 0.676 | 0.100 | 31 | 2.042 | 0.005 | 0.002 | 0.003 |
| 21 | 1.529 | 0.629 | 0.558 | 0.071 | 40 | 2.503 | 0.003 | 0.000 | 0.003 |
| 22 | 1.580 | 0.416 | 0.425 | -0.008 | 5 | 0.709 | 0.003 | 0.000 | 0.003 |
| 23 | 1.632 | 0.201 | 0.296 | -0.096 | 4 | 0.658 | 0.001 | 0.000 | 0.001 |
| 24 | 1.683 | 0.072 | 0.193 | -0.120 | 30 | 1.990 | 0.005 | 0.004 | 0.001 |
| 25 | 1.734 | 0.023 | 0.117 | -0.094 | 3 | 0.607 | 0.001 | 0.000 | 0.000 |
| 26 | 1.785 | 0.011 | 0.066 | -0.056 | 2 | 0.555 | 0.000 | 0.000 | 0.000 |
| 27 | 1.837 | 0.007 | 0.035 | -0.027 | 1 | 0.504 | 0.000 | 0.000 | 0.000 |
| 28 | 1.888 | 0.006 | 0.017 | -0.012 | 11 | 1.017 | 0.053 | 0.055 | -0.002 |
| 29 | 1.939 | 0.005 | 0.008 | -0.003 | 29 | 1.939 | 0.005 | 0.008 | -0.003 |
| 30 | 1.990 | 0.005 | 0.004 | 0.001 | 22 | 1.580 | 0.416 | 0.425 | -0.008 |
| 31 | 2.042 | 0.005 | 0.002 | 0.003 | 28 | 1.888 | 0.006 | 0.017 | -0.012 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 2.093 | 0.005 | 0.001 | 0.004 | 27 | 1.837 | 0.007 | 0.035 | -0.027 |
| 33 | 2.144 | 0.005 | 0.000 | 0.005 | 12 | 1.068 | 0.082 | 0.121 | -0.039 |
| 34 | 2.195 | 0.005 | 0.000 | 0.005 | 15 | 1.222 | 0.447 | 0.502 | -0.055 |
| 35 | 2.247 | 0.005 | 0.000 | 0.005 | 26 | 1.785 | 0.011 | 0.066 | -0.056 |
| 36 | 2.298 | 0.005 | 0.000 | 0.005 | 13 | 1.119 | 0.141 | 0.223 | -0.082 |
| 37 | 2.349 | 0.004 | 0.000 | 0.004 | 14 | 1.170 | 0.264 | 0.355 | -0.091 |
| 38 | 2.400 | 0.004 | 0.000 | 0.004 | 25 | 1.734 | 0.023 | 0.117 | -0.094 |
| 39 | 2.452 | 0.003 | 0.000 | 0.003 | 23 | 1.632 | 0.201 | 0.296 | -0.096 |
| 40 | 2.503 | 0.003 | 0.000 | 0.003 | 24 | 1.683 | 0.072 | 0.193 | -0.120 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 5% Methanol/95% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 305.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.309 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.6060 | 0.0003 |
| 2 | 0.6580 | 0.0007 |
| 3 | 0.7090 | 0.0019 |
| 4 | 0.7600 | 0.0041 |
| 5 | 0.8110 | 0.0077 |
| 6 | 0.8630 | 0.0133 |
| 7 | 0.9140 | 0.0218 |
| 8 | 0.9650 | 0.0338 |
| 9 | 1.0160 | 0.0499 |
| 10 | 1.0680 | 0.0785 |
| 11 | 1.1190 | 0.1387 |
| 12 | 1.1700 | 0.2247 |
| 13 | 1.2210 | 0.3449 |
| 14 | 1.2730 | 0.5036 |
| 15 | 1.3240 | 0.7017 |
| 16 | 1.3750 | 0.8171 |
| 17 | 1.4260 | 0.8316 |
| 18 | 1.4780 | 0.7858 |
| 19 | 1.5290 | 0.6491 |
| 20 | 1.5800 | 0.3957 |
| 21 | 1.6310 | 0.1656 |
| 22 | 1.6830 | 0.0522 |
| 23 | 1.7340 | 0.0200 |
| 24 | 1.7850 | 0.0109 |
| 25 | 1.8360 | 0.0070 |
| 26 | 1.8880 | 0.0055 |
| 27 | 1.9390 | 0.0047 |
| 28 | 1.9900 | 0.0041 |
| 29 | 2.0410 | 0.0038 |
| 30 | 2.0930 | 0.0036 |
| 31 | 2.1440 | 0.0034 |
| 32 | 2.1950 | 0.0032 |
| 33 | 2.2460 | 0.0031 |
| 34 | 2.2980 | 0.0029 |
| 35 | 2.3490 | 0.0028 |
| 36 | 2.4000 | 0.0027 |
| 37 | 2.4510 | 0.0026 |
| 38 | 2.5030 | 0.0027 |

| | | |
|---|---|---|
| 39 | 2.5540 | 0.0025 |
| 40 | 2.6050 | 0.0023 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 4.4736667 | 1.00000 |
| 1 | 2.1920920 | 1.09357 |
| 2 | 0.3298729 | 1.19663 |
| 3 | 0.0400964 | 1.24727 |
| 4 | 0.0381951 | 1.25170 |
| 5 | 0.0381951 | 1.25171 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.25171 | 0.0032 | 394.36 | 1.2453 | 1.2581 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.606 | 0.000 | 0.000 | 0.000 | 11 | 1.119 | 0.139 | 0.083 | 0.056 |
| 2 | 0.658 | 0.001 | 0.000 | 0.001 | 10 | 1.068 | 0.079 | 0.025 | 0.054 |
| 3 | 0.709 | 0.002 | 0.000 | 0.002 | 9 | 1.016 | 0.050 | 0.005 | 0.045 |
| 4 | 0.760 | 0.004 | 0.000 | 0.004 | 8 | 0.965 | 0.034 | 0.001 | 0.033 |
| 5 | 0.811 | 0.008 | 0.000 | 0.008 | 19 | 1.529 | 0.649 | 0.618 | 0.031 |
| 6 | 0.863 | 0.013 | 0.000 | 0.013 | 12 | 1.170 | 0.225 | 0.202 | 0.023 |
| 7 | 0.914 | 0.022 | 0.000 | 0.022 | 7 | 0.914 | 0.022 | 0.000 | 0.022 |
| 8 | 0.965 | 0.034 | 0.001 | 0.033 | 6 | 0.863 | 0.013 | 0.000 | 0.013 |
| 9 | 1.016 | 0.050 | 0.005 | 0.045 | 5 | 0.811 | 0.008 | 0.000 | 0.008 |
| 10 | 1.068 | 0.079 | 0.025 | 0.054 | 18 | 1.478 | 0.786 | 0.781 | 0.004 |
| 11 | 1.119 | 0.139 | 0.083 | 0.056 | 27 | 1.939 | 0.005 | 0.001 | 0.004 |
| 12 | 1.170 | 0.225 | 0.202 | 0.023 | 4 | 0.760 | 0.004 | 0.000 | 0.004 |
| 13 | 1.221 | 0.345 | 0.379 | -0.034 | 28 | 1.990 | 0.004 | 0.000 | 0.004 |
| 14 | 1.273 | 0.504 | 0.582 | -0.078 | 29 | 2.041 | 0.004 | 0.000 | 0.004 |
| 15 | 1.324 | 0.702 | 0.752 | -0.050 | 30 | 2.093 | 0.004 | 0.000 | 0.004 |
| 16 | 1.375 | 0.817 | 0.854 | -0.037 | 26 | 1.888 | 0.005 | 0.002 | 0.004 |
| 17 | 1.426 | 0.832 | 0.867 | -0.036 | 31 | 2.144 | 0.003 | 0.000 | 0.003 |
| 18 | 1.478 | 0.786 | 0.781 | 0.004 | 32 | 2.195 | 0.003 | 0.000 | 0.003 |
| 19 | 1.529 | 0.649 | 0.618 | 0.031 | 33 | 2.246 | 0.003 | 0.000 | 0.003 |
| 20 | 1.580 | 0.396 | 0.423 | -0.027 | 34 | 2.298 | 0.003 | 0.000 | 0.003 |
| 21 | 1.631 | 0.166 | 0.249 | -0.084 | 35 | 2.349 | 0.003 | 0.000 | 0.003 |
| 22 | 1.683 | 0.052 | 0.124 | -0.072 | 38 | 2.503 | 0.003 | 0.000 | 0.003 |
| 23 | 1.734 | 0.020 | 0.054 | -0.034 | 36 | 2.400 | 0.003 | 0.000 | 0.003 |
| 24 | 1.785 | 0.011 | 0.021 | -0.010 | 37 | 2.451 | 0.003 | 0.000 | 0.003 |
| 25 | 1.836 | 0.007 | 0.007 | 0.000 | 39 | 2.554 | 0.003 | 0.000 | 0.002 |
| 26 | 1.888 | 0.005 | 0.002 | 0.004 | 40 | 2.605 | 0.002 | 0.000 | 0.002 |
| 27 | 1.939 | 0.005 | 0.001 | 0.004 | 3 | 0.709 | 0.002 | 0.000 | 0.002 |
| 28 | 1.990 | 0.004 | 0.000 | 0.004 | 2 | 0.658 | 0.001 | 0.000 | 0.001 |
| 29 | 2.041 | 0.004 | 0.000 | 0.004 | 1 | 0.606 | 0.000 | 0.000 | 0.000 |
| 30 | 2.093 | 0.004 | 0.000 | 0.004 | 25 | 1.836 | 0.007 | 0.007 | 0.000 |
| 31 | 2.144 | 0.003 | 0.000 | 0.003 | 24 | 1.785 | 0.011 | 0.021 | -0.010 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 2.195 | 0.003 | 0.000 | 0.003 | 20 | 1.580 | 0.396 | 0.423 | -0.027 |
| 33 | 2.246 | 0.003 | 0.000 | 0.003 | 23 | 1.734 | 0.020 | 0.054 | -0.034 |
| 34 | 2.298 | 0.003 | 0.000 | 0.003 | 13 | 1.221 | 0.345 | 0.379 | -0.034 |
| 35 | 2.349 | 0.003 | 0.000 | 0.003 | 17 | 1.426 | 0.832 | 0.867 | -0.036 |
| 36 | 2.400 | 0.003 | 0.000 | 0.003 | 16 | 1.375 | 0.817 | 0.854 | -0.037 |
| 37 | 2.451 | 0.003 | 0.000 | 0.003 | 15 | 1.324 | 0.702 | 0.752 | -0.050 |
| 38 | 2.503 | 0.003 | 0.000 | 0.003 | 22 | 1.683 | 0.052 | 0.124 | -0.072 |
| 39 | 2.554 | 0.003 | 0.000 | 0.002 | 14 | 1.273 | 0.504 | 0.582 | -0.078 |
| 40 | 2.605 | 0.002 | 0.000 | 0.002 | 21 | 1.631 | 0.166 | 0.249 | -0.084 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 10% Methanol/90% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 276.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.320 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4500 | 0.0002 |
| 2 | 0.5010 | 0.0007 |
| 3 | 0.5530 | 0.0018 |
| 4 | 0.6040 | 0.0044 |
| 5 | 0.6550 | 0.0077 |
| 6 | 0.7060 | 0.0122 |
| 7 | 0.7580 | 0.0181 |
| 8 | 0.8090 | 0.0242 |
| 9 | 0.8600 | 0.0328 |
| 10 | 0.9110 | 0.0406 |
| 11 | 0.9630 | 0.0507 |
| 12 | 1.0140 | 0.0659 |
| 13 | 1.0650 | 0.0934 |
| 14 | 1.1160 | 0.1523 |
| 15 | 1.1680 | 0.2284 |
| 16 | 1.2190 | 0.3264 |
| 17 | 1.2700 | 0.5001 |
| 18 | 1.3210 | 0.6810 |
| 19 | 1.3730 | 0.7971 |
| 20 | 1.4240 | 0.8124 |
| 21 | 1.4750 | 0.7504 |
| 22 | 1.5260 | 0.6556 |
| 23 | 1.5780 | 0.4617 |
| 24 | 1.6290 | 0.2220 |
| 25 | 1.6800 | 0.0719 |
| 26 | 1.7310 | 0.0266 |
| 27 | 1.7830 | 0.0139 |
| 28 | 1.8340 | 0.0093 |
| 29 | 1.8850 | 0.0068 |
| 30 | 1.9360 | 0.0054 |
| 31 | 1.9880 | 0.0045 |
| 32 | 2.0390 | 0.0038 |
| 33 | 2.0900 | 0.0033 |
| 34 | 2.1410 | 0.0029 |
| 35 | 2.1930 | 0.0026 |
| 36 | 2.2440 | 0.0024 |
| 37 | 2.2950 | 0.0022 |
| 38 | 2.3460 | 0.0021 |

| | | |
|---|---|---|
| 39 | 2.3980 | 0.0020 |
| 40 | 2.4490 | 0.0019 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 4.1831929 | 1.00000 |
| 1 | 1.9238347 | 1.09672 |
| 2 | 0.2849047 | 1.19765 |
| 3 | 0.0550446 | 1.24384 |
| 4 | 0.0528172 | 1.24887 |
| 5 | 0.0528172 | 1.24887 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.24887 | 0.0038 | 325.63 | 1.2411 | 1.2566 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.450 | 0.000 | 0.000 | 0.000 | 13 | 1.065 | 0.093 | 0.030 | 0.063 |
| 2 | 0.501 | 0.001 | 0.000 | 0.001 | 14 | 1.116 | 0.152 | 0.093 | 0.060 |
| 3 | 0.553 | 0.002 | 0.000 | 0.002 | 12 | 1.014 | 0.066 | 0.007 | 0.059 |
| 4 | 0.604 | 0.004 | 0.000 | 0.004 | 11 | 0.963 | 0.051 | 0.001 | 0.050 |
| 5 | 0.655 | 0.008 | 0.000 | 0.008 | 10 | 0.911 | 0.041 | 0.000 | 0.041 |
| 6 | 0.706 | 0.012 | 0.000 | 0.012 | 9 | 0.860 | 0.033 | 0.000 | 0.033 |
| 7 | 0.758 | 0.018 | 0.000 | 0.018 | 8 | 0.809 | 0.024 | 0.000 | 0.024 |
| 8 | 0.809 | 0.024 | 0.000 | 0.024 | 7 | 0.758 | 0.018 | 0.000 | 0.018 |
| 9 | 0.860 | 0.033 | 0.000 | 0.033 | 15 | 1.168 | 0.228 | 0.215 | 0.013 |
| 10 | 0.911 | 0.041 | 0.000 | 0.041 | 6 | 0.706 | 0.012 | 0.000 | 0.012 |
| 11 | 0.963 | 0.051 | 0.001 | 0.050 | 5 | 0.655 | 0.008 | 0.000 | 0.008 |
| 12 | 1.014 | 0.066 | 0.007 | 0.059 | 22 | 1.526 | 0.656 | 0.650 | 0.005 |
| 13 | 1.065 | 0.093 | 0.030 | 0.063 | 4 | 0.604 | 0.004 | 0.000 | 0.004 |
| 14 | 1.116 | 0.152 | 0.093 | 0.060 | 30 | 1.936 | 0.005 | 0.001 | 0.004 |
| 15 | 1.168 | 0.228 | 0.215 | 0.013 | 31 | 1.988 | 0.004 | 0.000 | 0.004 |
| 16 | 1.219 | 0.326 | 0.388 | -0.061 | 32 | 2.039 | 0.004 | 0.000 | 0.004 |
| 17 | 1.270 | 0.500 | 0.578 | -0.077 | 33 | 2.090 | 0.003 | 0.000 | 0.003 |
| 18 | 1.321 | 0.681 | 0.741 | -0.060 | 29 | 1.885 | 0.007 | 0.004 | 0.003 |
| 19 | 1.373 | 0.797 | 0.845 | -0.048 | 34 | 2.141 | 0.003 | 0.000 | 0.003 |
| 20 | 1.424 | 0.812 | 0.866 | -0.053 | 35 | 2.193 | 0.003 | 0.000 | 0.003 |
| 21 | 1.475 | 0.750 | 0.796 | -0.046 | 36 | 2.244 | 0.002 | 0.000 | 0.002 |
| 22 | 1.526 | 0.656 | 0.650 | 0.005 | 37 | 2.295 | 0.002 | 0.000 | 0.002 |
| 23 | 1.578 | 0.462 | 0.463 | -0.001 | 38 | 2.346 | 0.002 | 0.000 | 0.002 |
| 24 | 1.629 | 0.222 | 0.289 | -0.067 | 39 | 2.398 | 0.002 | 0.000 | 0.002 |
| 25 | 1.680 | 0.072 | 0.158 | -0.086 | 40 | 2.449 | 0.002 | 0.000 | 0.002 |
| 26 | 1.731 | 0.027 | 0.075 | -0.049 | 3 | 0.553 | 0.002 | 0.000 | 0.002 |
| 27 | 1.783 | 0.014 | 0.031 | -0.017 | 2 | 0.501 | 0.001 | 0.000 | 0.001 |
| 28 | 1.834 | 0.009 | 0.012 | -0.002 | 1 | 0.450 | 0.000 | 0.000 | 0.000 |
| 29 | 1.885 | 0.007 | 0.004 | 0.003 | 23 | 1.578 | 0.462 | 0.463 | -0.001 |
| 30 | 1.936 | 0.005 | 0.001 | 0.004 | 28 | 1.834 | 0.009 | 0.012 | -0.002 |
| 31 | 1.988 | 0.004 | 0.000 | 0.004 | 27 | 1.783 | 0.014 | 0.031 | -0.017 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 32 | 2.039 | 0.004 | 0.000 | 0.004 | 21 | 1.475 | 0.750 | 0.796 | -0.046 |
| 33 | 2.090 | 0.003 | 0.000 | 0.003 | 19 | 1.373 | 0.797 | 0.845 | -0.048 |
| 34 | 2.141 | 0.003 | 0.000 | 0.003 | 26 | 1.731 | 0.027 | 0.075 | -0.049 |
| 35 | 2.193 | 0.003 | 0.000 | 0.003 | 20 | 1.424 | 0.812 | 0.866 | -0.053 |
| 36 | 2.244 | 0.002 | 0.000 | 0.002 | 18 | 1.321 | 0.681 | 0.741 | -0.060 |
| 37 | 2.295 | 0.002 | 0.000 | 0.002 | 16 | 1.219 | 0.326 | 0.388 | -0.061 |
| 38 | 2.346 | 0.002 | 0.000 | 0.002 | 24 | 1.629 | 0.222 | 0.289 | -0.067 |
| 39 | 2.398 | 0.002 | 0.000 | 0.002 | 17 | 1.270 | 0.500 | 0.578 | -0.077 |
| 40 | 2.449 | 0.002 | 0.000 | 0.002 | 25 | 1.680 | 0.072 | 0.158 | -0.086 |

END OF PROBLEM

1

**********

NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 20% Methanol/80% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 328.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.313 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4830 | 0.0125 |
| 2 | 0.5350 | 0.0172 |
| 3 | 0.5860 | 0.0221 |
| 4 | 0.6370 | 0.0276 |
| 5 | 0.6880 | 0.0330 |
| 6 | 0.7400 | 0.0374 |
| 7 | 0.7910 | 0.0444 |
| 8 | 0.8420 | 0.0516 |
| 9 | 0.8930 | 0.0607 |
| 10 | 0.9450 | 0.0735 |
| 11 | 0.9960 | 0.0930 |
| 12 | 1.0470 | 0.1491 |
| 13 | 1.0980 | 0.2285 |
| 14 | 1.1500 | 0.3114 |
| 15 | 1.2010 | 0.3575 |
| 16 | 1.2520 | 0.4748 |
| 17 | 1.3030 | 0.6591 |
| 18 | 1.3550 | 0.8305 |
| 19 | 1.4060 | 0.8706 |
| 20 | 1.4570 | 0.7595 |
| 21 | 1.5080 | 0.6463 |
| 22 | 1.5600 | 0.4454 |
| 23 | 1.6110 | 0.2223 |
| 24 | 1.6620 | 0.0708 |
| 25 | 1.7130 | 0.0333 |
| 26 | 1.7650 | 0.0120 |
| 27 | 1.8160 | 0.0140 |
| 28 | 1.8670 | 0.0111 |
| 29 | 1.9180 | 0.0092 |
| 30 | 1.9700 | 0.0075 |
| 31 | 2.0210 | 0.0072 |
| 32 | 2.0720 | 0.0056 |
| 33 | 2.1230 | 0.0052 |
| 34 | 2.1750 | 0.0047 |
| 35 | 2.2260 | 0.0046 |
| 36 | 2.2770 | 0.0044 |
| 37 | 2.3280 | 0.0043 |
| 38 | 2.3800 | 0.0044 |

| | | |
|---|---|---|
| 39 | 2.4310 | 0.0043 |
| 40 | 2.4820 | 0.0040 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 3.7921204 | 1.00000 |
| 1 | 1.8465650 | 1.08619 |
| 2 | 0.4169640 | 1.17352 |
| 3 | 0.1260098 | 1.22018 |
| 4 | 0.1150433 | 1.23034 |
| 5 | 0.1150326 | 1.23175 |
| 6 | 0.1150326 | 1.23175 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.23175 | 0.0053 | 233.02 | 1.2211 | 1.2424 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.483 | 0.013 | 0.000 | 0.013 | 13 | 1.098 | 0.229 | 0.070 | 0.158 |
| 2 | 0.535 | 0.017 | 0.000 | 0.017 | 12 | 1.047 | 0.149 | 0.018 | 0.131 |
| 3 | 0.586 | 0.022 | 0.000 | 0.022 | 14 | 1.150 | 0.311 | 0.189 | 0.122 |
| 4 | 0.637 | 0.028 | 0.000 | 0.028 | 11 | 0.996 | 0.093 | 0.003 | 0.090 |
| 5 | 0.688 | 0.033 | 0.000 | 0.033 | 10 | 0.945 | 0.073 | 0.000 | 0.073 |
| 6 | 0.740 | 0.037 | 0.000 | 0.037 | 9 | 0.893 | 0.061 | 0.000 | 0.061 |
| 7 | 0.791 | 0.044 | 0.000 | 0.044 | 8 | 0.842 | 0.052 | 0.000 | 0.052 |
| 8 | 0.842 | 0.052 | 0.000 | 0.052 | 7 | 0.791 | 0.044 | 0.000 | 0.044 |
| 9 | 0.893 | 0.061 | 0.000 | 0.061 | 6 | 0.740 | 0.037 | 0.000 | 0.037 |
| 10 | 0.945 | 0.073 | 0.000 | 0.073 | 5 | 0.688 | 0.033 | 0.000 | 0.033 |
| 11 | 0.996 | 0.093 | 0.003 | 0.090 | 4 | 0.637 | 0.028 | 0.000 | 0.028 |
| 12 | 1.047 | 0.149 | 0.018 | 0.131 | 3 | 0.586 | 0.022 | 0.000 | 0.022 |
| 13 | 1.098 | 0.229 | 0.070 | 0.158 | 2 | 0.535 | 0.017 | 0.000 | 0.017 |
| 14 | 1.150 | 0.311 | 0.189 | 0.122 | 1 | 0.483 | 0.013 | 0.000 | 0.013 |
| 15 | 1.201 | 0.357 | 0.373 | -0.015 | 28 | 1.867 | 0.011 | 0.001 | 0.010 |
| 16 | 1.252 | 0.475 | 0.583 | -0.108 | 22 | 1.560 | 0.445 | 0.436 | 0.009 |
| 17 | 1.303 | 0.659 | 0.762 | -0.103 | 29 | 1.918 | 0.009 | 0.000 | 0.009 |
| 18 | 1.355 | 0.831 | 0.874 | -0.043 | 27 | 1.816 | 0.014 | 0.005 | 0.009 |
| 19 | 1.406 | 0.871 | 0.893 | -0.022 | 30 | 1.970 | 0.007 | 0.000 | 0.007 |
| 20 | 1.457 | 0.759 | 0.813 | -0.053 | 31 | 2.021 | 0.007 | 0.000 | 0.007 |
| 21 | 1.508 | 0.646 | 0.647 | 0.000 | 32 | 2.072 | 0.006 | 0.000 | 0.006 |
| 22 | 1.560 | 0.445 | 0.436 | 0.009 | 33 | 2.123 | 0.005 | 0.000 | 0.005 |
| 23 | 1.611 | 0.222 | 0.251 | -0.028 | 34 | 2.175 | 0.005 | 0.000 | 0.005 |
| 24 | 1.662 | 0.071 | 0.122 | -0.051 | 35 | 2.226 | 0.005 | 0.000 | 0.005 |
| 25 | 1.713 | 0.033 | 0.050 | -0.017 | 38 | 2.380 | 0.004 | 0.000 | 0.004 |
| 26 | 1.765 | 0.012 | 0.017 | -0.005 | 36 | 2.277 | 0.004 | 0.000 | 0.004 |
| 27 | 1.816 | 0.014 | 0.005 | 0.009 | 39 | 2.431 | 0.004 | 0.000 | 0.004 |
| 28 | 1.867 | 0.011 | 0.001 | 0.010 | 37 | 2.328 | 0.004 | 0.000 | 0.004 |
| 29 | 1.918 | 0.009 | 0.000 | 0.009 | 40 | 2.482 | 0.004 | 0.000 | 0.004 |
| 30 | 1.970 | 0.007 | 0.000 | 0.007 | 21 | 1.508 | 0.646 | 0.647 | 0.000 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 31 | 2.021 | 0.007 | 0.000 | 0.007 | 26 | 1.765 | 0.012 | 0.017 | -0.005 |
| 32 | 2.072 | 0.006 | 0.000 | 0.006 | 15 | 1.201 | 0.357 | 0.373 | -0.015 |
| 33 | 2.123 | 0.005 | 0.000 | 0.005 | 25 | 1.713 | 0.033 | 0.050 | -0.017 |
| 34 | 2.175 | 0.005 | 0.000 | 0.005 | 19 | 1.406 | 0.871 | 0.893 | -0.022 |
| 35 | 2.226 | 0.005 | 0.000 | 0.005 | 23 | 1.611 | 0.222 | 0.251 | -0.028 |
| 36 | 2.277 | 0.004 | 0.000 | 0.004 | 18 | 1.355 | 0.831 | 0.874 | -0.043 |
| 37 | 2.328 | 0.004 | 0.000 | 0.004 | 24 | 1.662 | 0.071 | 0.122 | -0.051 |
| 38 | 2.380 | 0.004 | 0.000 | 0.004 | 20 | 1.457 | 0.759 | 0.813 | -0.053 |
| 39 | 2.431 | 0.004 | 0.000 | 0.004 | 17 | 1.303 | 0.659 | 0.762 | -0.103 |
| 40 | 2.482 | 0.004 | 0.000 | 0.004 | 16 | 1.252 | 0.475 | 0.583 | -0.108 |

END OF PROBLEM

1

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NON-LINEAR LEAST SQUARES ANALYSIS

EQUILIBRIUM TRANSPORT (MODEL A)
THIRD-TYPE BOUNDARY CONDITION
PCE Run: 50% Methanol/50% Water

**********

INITIAL VALUES OF COEFFICIENTS

| NO | NAME | INITIAL VALUE |
|---|---|---|
| 1 | PECLET | 221.000 |
| 2 | RF | 1.000 |
| 3 | PUL | 0.326 |

OBSERVED DATA

| OBS. NO. | PORE VOLUME | CONCENTRATION |
|---|---|---|
| 1 | 0.4330 | 0.0084 |
| 2 | 0.4850 | 0.0136 |
| 3 | 0.5360 | 0.0191 |
| 4 | 0.5870 | 0.0237 |
| 5 | 0.6380 | 0.0296 |
| 6 | 0.6900 | 0.0352 |
| 7 | 0.7410 | 0.0384 |
| 8 | 0.7920 | 0.0453 |
| 9 | 0.8430 | 0.0511 |
| 10 | 0.8950 | 0.0757 |
| 11 | 0.9460 | 0.0688 |
| 12 | 0.9970 | 0.0902 |
| 13 | 1.0480 | 0.1298 |
| 14 | 1.1000 | 0.2016 |
| 15 | 1.1510 | 0.2740 |
| 16 | 1.2020 | 0.3354 |
| 17 | 1.2530 | 0.4179 |
| 18 | 1.3050 | 0.5865 |
| 19 | 1.3560 | 0.8007 |
| 20 | 1.4070 | 0.9018 |
| 21 | 1.4580 | 0.8672 |
| 22 | 1.5100 | 0.7320 |
| 23 | 1.5610 | 0.4621 |
| 24 | 1.6120 | 0.2397 |
| 25 | 1.6630 | 0.1438 |
| 26 | 1.7150 | 0.0839 |
| 27 | 1.7660 | 0.0619 |
| 28 | 1.8170 | 0.0458 |
| 29 | 1.8680 | 0.0300 |
| 30 | 1.9200 | 0.0191 |
| 31 | 1.9710 | 0.0122 |
| 32 | 2.0220 | 0.0083 |
| 33 | 2.0730 | 0.0057 |
| 34 | 2.1250 | 0.0048 |
| 35 | 2.1760 | 0.0039 |
| 36 | 2.2270 | 0.0034 |
| 37 | 2.2780 | 0.0030 |
| 38 | 2.3300 | 0.0026 |

| | | |
|---|---|---|
| 39 | 2.3810 | 0.0024 |
| 40 | 2.4320 | 0.0022 |

| ITERATION | SSQ | RF |
|---|---|---|
| 0 | 3.8082657 | 1.00000 |
| 1 | 1.5077115 | 1.10596 |
| 2 | 0.1944039 | 1.20882 |
| 3 | 0.1126366 | 1.23999 |
| 4 | 0.1126193 | 1.24035 |

1 CORRELATION MATRIX

| | 1 |
|---|---|
| 1 | 1.0000 |

NON-LINEAR LEAST SQUARES ANALYSIS, FINAL RESULTS

| VARIABLE | NAME | VALUE | S.E.COEFF. | T-VALUE | 95% CONFIDENCE LIMITS LOWER | UPPER |
|---|---|---|---|---|---|---|
| 1 | RF | 1.24035 | 0.0061 | 204.98 | 1.2281 | 1.2526 |

| -----ORDERED BY COMPUTER INPUT----- | | | | | -----ORDERED BY RESIDUALS----- | | | | |
|---|---|---|---|---|---|---|---|---|---|
| PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL | PORE NO | CONCENTRATION VOLUME | OBS. | FITTED | RESI-DUAL |
| 1 | 0.433 | 0.008 | 0.000 | 0.008 | 14 | 1.100 | 0.202 | 0.103 | 0.099 |
| 2 | 0.485 | 0.014 | 0.000 | 0.014 | 13 | 1.048 | 0.130 | 0.038 | 0.092 |
| 3 | 0.536 | 0.019 | 0.000 | 0.019 | 12 | 0.997 | 0.090 | 0.011 | 0.080 |
| 4 | 0.587 | 0.024 | 0.000 | 0.024 | 21 | 1.458 | 0.867 | 0.788 | 0.079 |
| 5 | 0.638 | 0.030 | 0.000 | 0.030 | 10 | 0.895 | 0.076 | 0.000 | 0.075 |
| 6 | 0.690 | 0.035 | 0.000 | 0.035 | 20 | 1.407 | 0.902 | 0.835 | 0.067 |
| 7 | 0.741 | 0.038 | 0.000 | 0.038 | 11 | 0.946 | 0.069 | 0.002 | 0.067 |
| 8 | 0.792 | 0.045 | 0.000 | 0.045 | 22 | 1.510 | 0.732 | 0.669 | 0.063 |
| 9 | 0.843 | 0.051 | 0.000 | 0.051 | 15 | 1.151 | 0.274 | 0.215 | 0.059 |
| 10 | 0.895 | 0.076 | 0.000 | 0.075 | 9 | 0.843 | 0.051 | 0.000 | 0.051 |
| 11 | 0.946 | 0.069 | 0.002 | 0.067 | 8 | 0.792 | 0.045 | 0.000 | 0.045 |
| 12 | 0.997 | 0.090 | 0.011 | 0.080 | 7 | 0.741 | 0.038 | 0.000 | 0.038 |
| 13 | 1.048 | 0.130 | 0.038 | 0.092 | 6 | 0.690 | 0.035 | 0.000 | 0.035 |
| 14 | 1.100 | 0.202 | 0.103 | 0.099 | 5 | 0.638 | 0.030 | 0.000 | 0.030 |
| 15 | 1.151 | 0.274 | 0.215 | 0.059 | 4 | 0.587 | 0.024 | 0.000 | 0.024 |
| 16 | 1.202 | 0.335 | 0.370 | -0.035 | 28 | 1.817 | 0.046 | 0.026 | 0.020 |
| 17 | 1.253 | 0.418 | 0.541 | -0.124 | 29 | 1.868 | 0.030 | 0.011 | 0.019 |
| 18 | 1.305 | 0.587 | 0.698 | -0.111 | 3 | 0.536 | 0.019 | 0.000 | 0.019 |
| 19 | 1.356 | 0.801 | 0.801 | -0.001 | 30 | 1.920 | 0.019 | 0.004 | 0.015 |
| 20 | 1.407 | 0.902 | 0.835 | 0.067 | 2 | 0.485 | 0.014 | 0.000 | 0.014 |
| 21 | 1.458 | 0.867 | 0.788 | 0.079 | 31 | 1.971 | 0.012 | 0.001 | 0.011 |
| 22 | 1.510 | 0.732 | 0.669 | 0.063 | 1 | 0.433 | 0.008 | 0.000 | 0.008 |
| 23 | 1.561 | 0.462 | 0.511 | -0.049 | 32 | 2.022 | 0.008 | 0.000 | 0.008 |
| 24 | 1.612 | 0.240 | 0.349 | -0.109 | 33 | 2.073 | 0.006 | 0.000 | 0.006 |
| 25 | 1.663 | 0.144 | 0.214 | -0.070 | 34 | 2.125 | 0.005 | 0.000 | 0.005 |
| 26 | 1.715 | 0.084 | 0.116 | -0.032 | 27 | 1.766 | 0.062 | 0.058 | 0.004 |
| 27 | 1.766 | 0.062 | 0.058 | 0.004 | 35 | 2.176 | 0.004 | 0.000 | 0.004 |
| 28 | 1.817 | 0.046 | 0.026 | 0.020 | 36 | 2.227 | 0.003 | 0.000 | 0.003 |
| 29 | 1.868 | 0.030 | 0.011 | 0.019 | 37 | 2.278 | 0.003 | 0.000 | 0.003 |
| 30 | 1.920 | 0.019 | 0.004 | 0.015 | 38 | 2.330 | 0.003 | 0.000 | 0.003 |
| 31 | 1.971 | 0.012 | 0.001 | 0.011 | 39 | 2.381 | 0.002 | 0.000 | 0.002 |
| 32 | 2.022 | 0.008 | 0.000 | 0.008 | 40 | 2.432 | 0.002 | 0.000 | 0.002 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 33 | 2.073 | 0.006 | 0.000 | 0.006 | 19 | 1.356 | 0.801 | 0.801 | -0.001 |
| 34 | 2.125 | 0.005 | 0.000 | 0.005 | 26 | 1.715 | 0.084 | 0.116 | -0.032 |
| 35 | 2.176 | 0.004 | 0.000 | 0.004 | 16 | 1.202 | 0.335 | 0.370 | -0.035 |
| 36 | 2.227 | 0.003 | 0.000 | 0.003 | 23 | 1.561 | 0.462 | 0.511 | -0.049 |
| 37 | 2.278 | 0.003 | 0.000 | 0.003 | 25 | 1.663 | 0.144 | 0.214 | -0.070 |
| 38 | 2.330 | 0.003 | 0.000 | 0.003 | 24 | 1.612 | 0.240 | 0.349 | -0.109 |
| 39 | 2.381 | 0.002 | 0.000 | 0.002 | 18 | 1.305 | 0.587 | 0.698 | -0.111 |
| 40 | 2.432 | 0.002 | 0.000 | 0.002 | 17 | 1.253 | 0.418 | 0.541 | -0.124 |

END OF PROBLEM

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